

## SUPPORTING INFORMATION

### Synthesis of 2-Tetrazolylmethyl-isoindolin-1-ones via a One Pot Ugi-Azide/(N-Acylation/ *exo* Diels–Alder)/Dehydration Process

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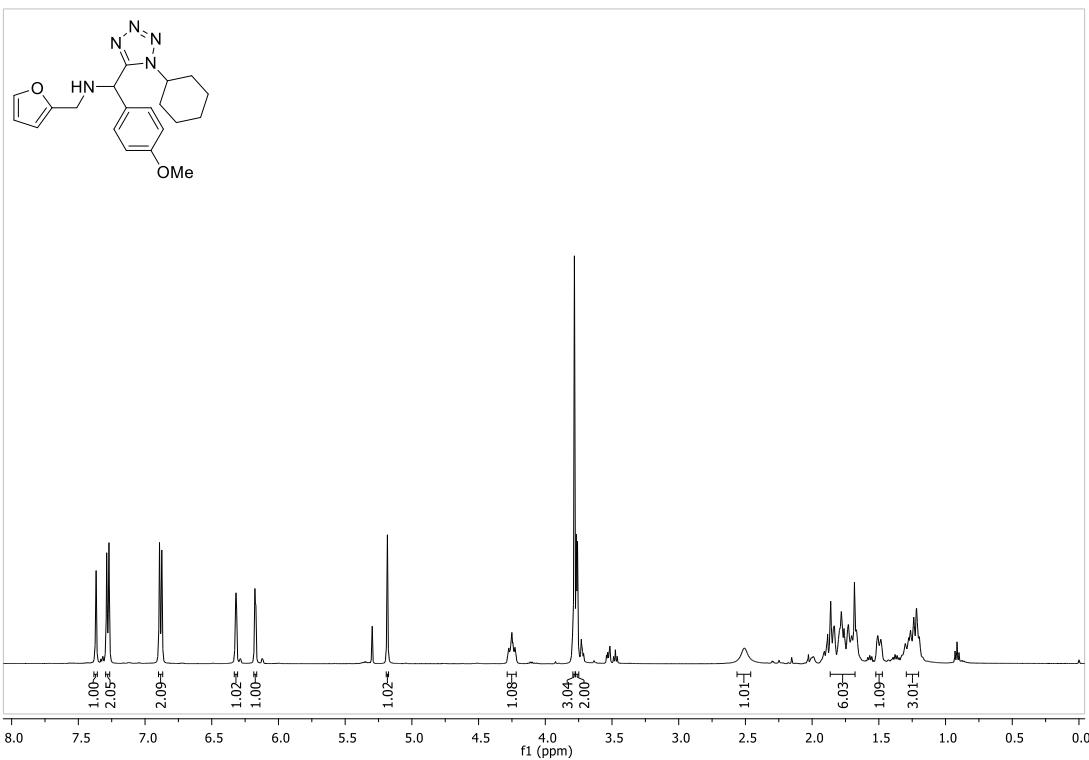
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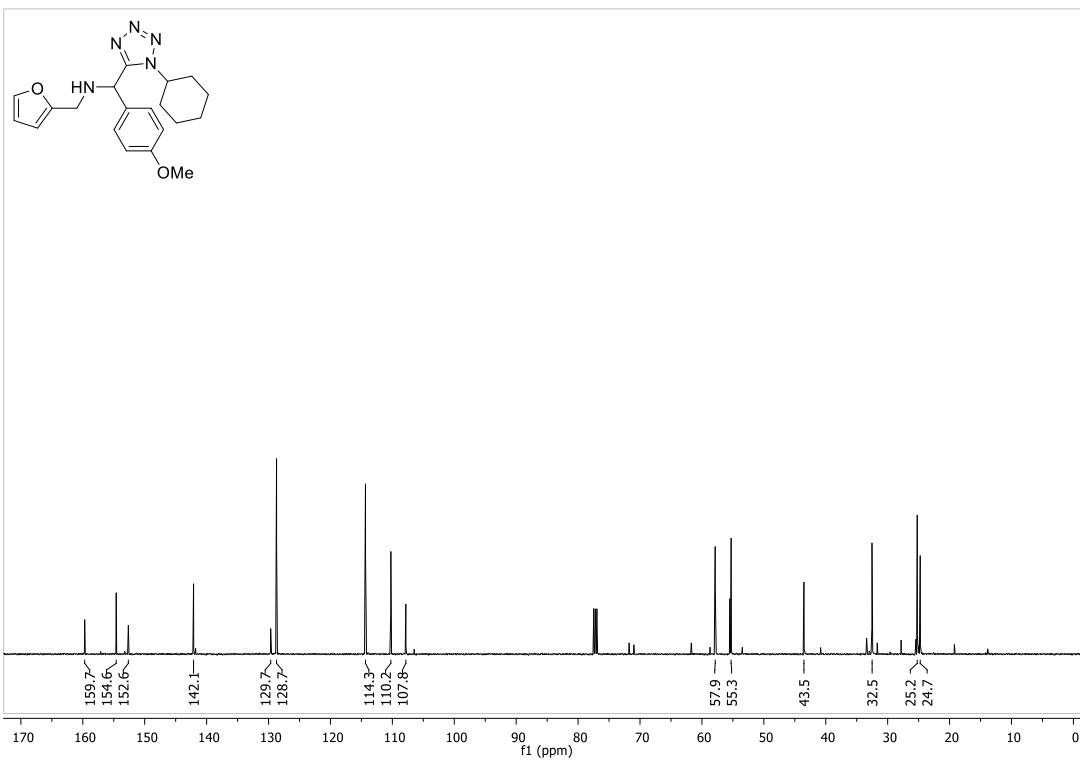
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#### Table of Contents

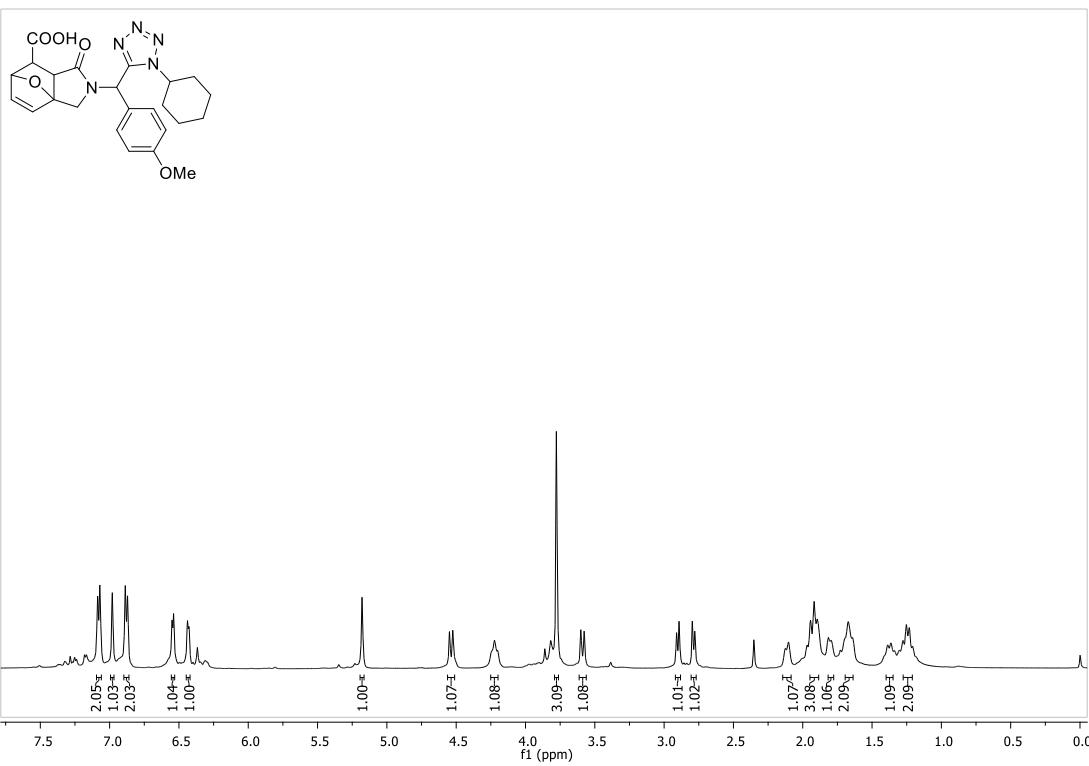
Supporting information for the product <b>6a</b> .....	S2
Supporting information for the product <b>8a</b> .....	S3
Supporting information for the products <b>1a-o</b> .....	S4-S20
Computational Study.....	S21-S63



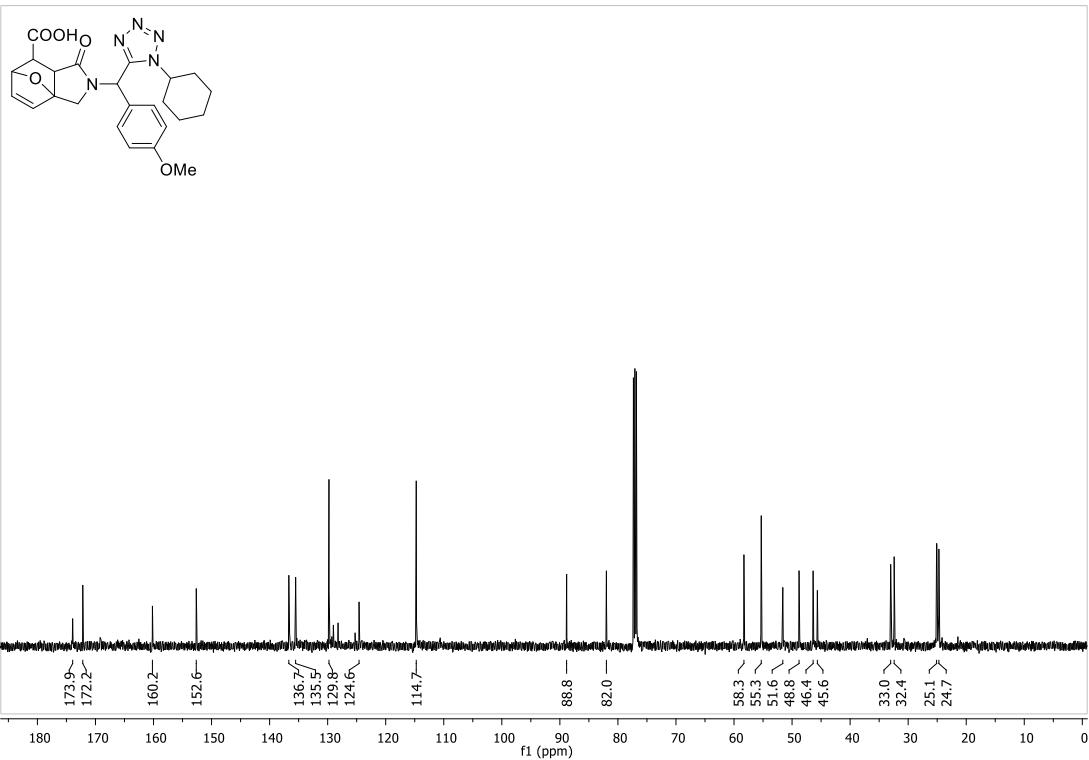
**Figure S1.** <sup>1</sup>H NMR spectrum of the compound 6a



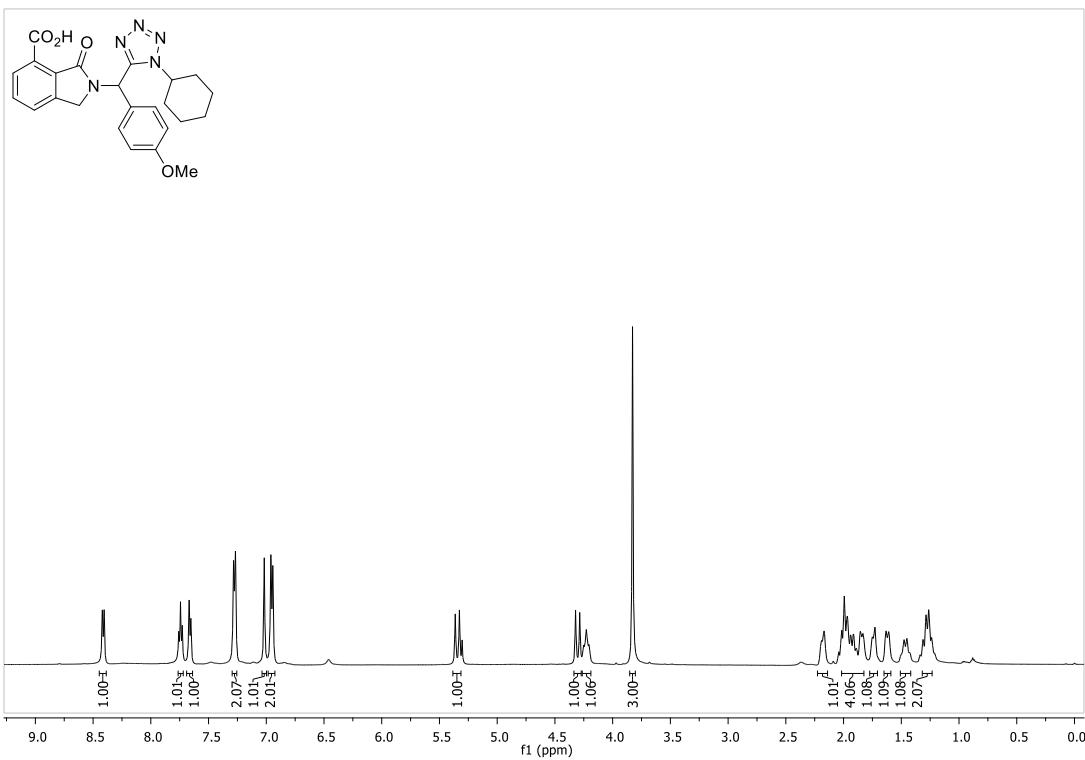
**Figure S2.** <sup>13</sup>C NMR spectrum of the compound 6a



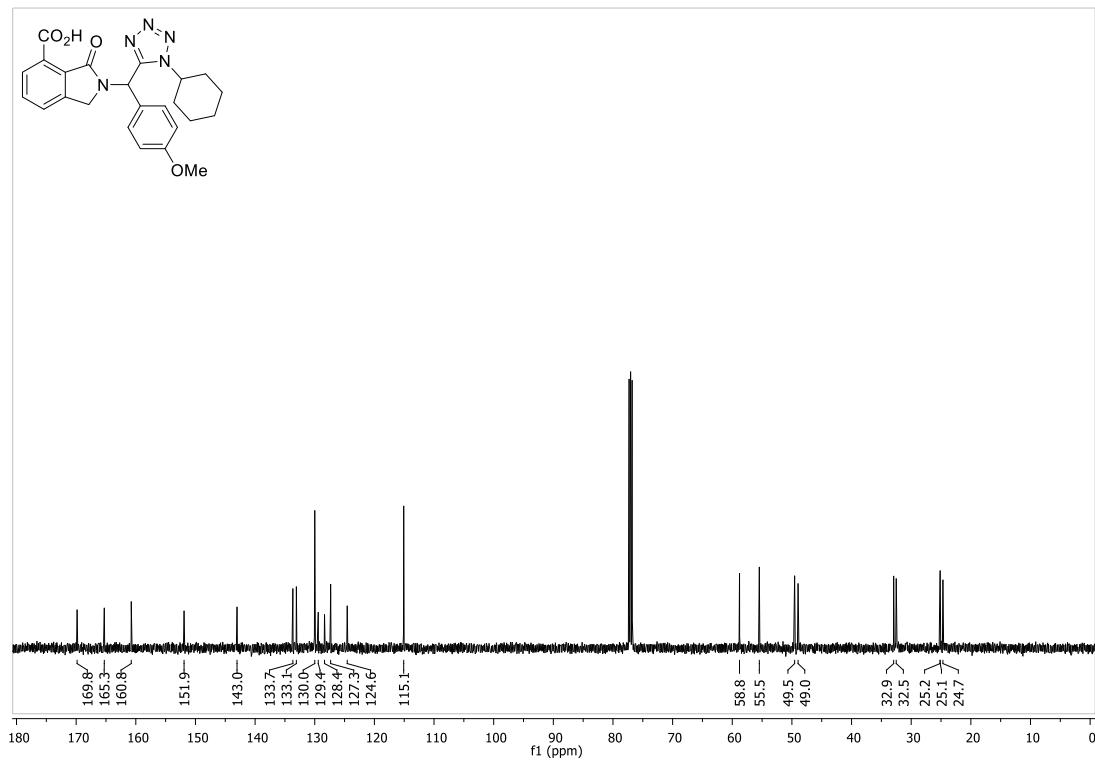
**Figure S4.** <sup>1</sup>H NMR spectrum of the compound 8a



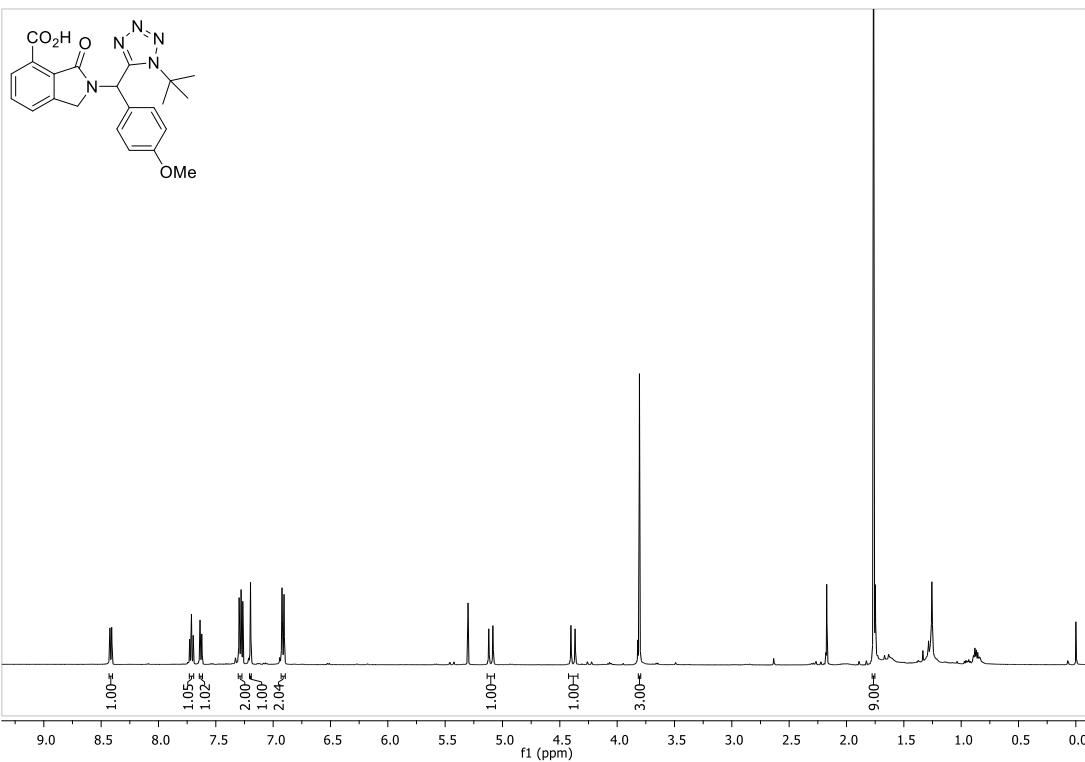
**Figure S4.** <sup>13</sup>C NMR spectrum of the compound 8a



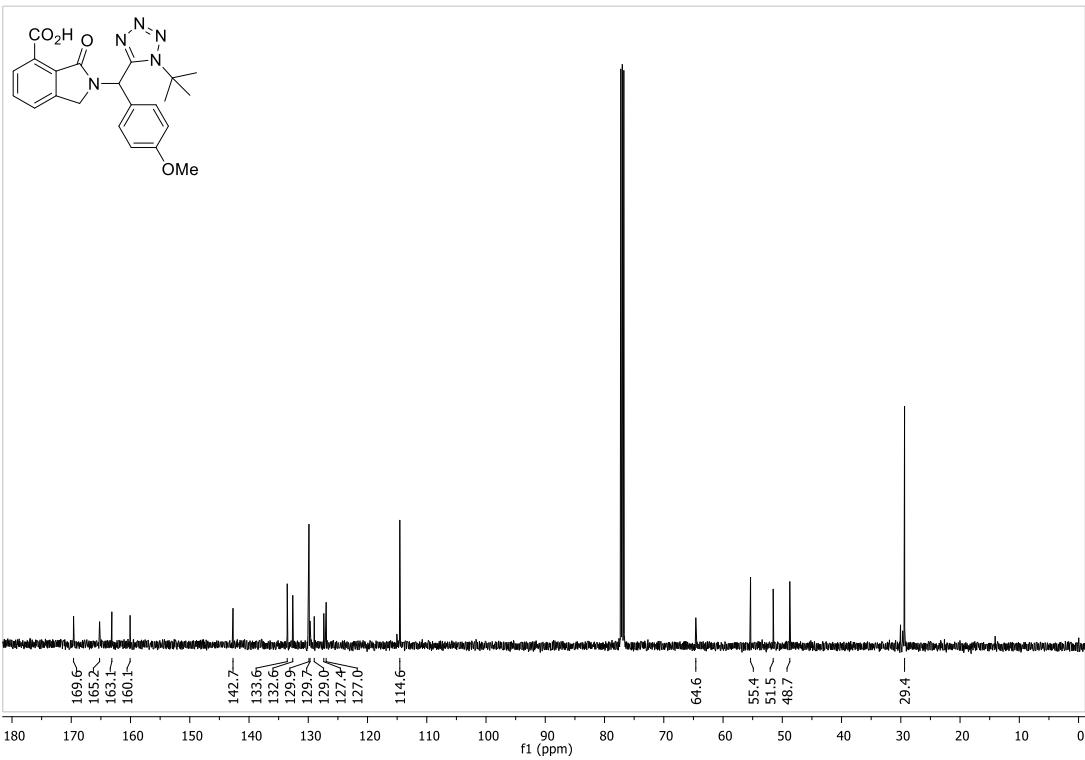
**Figure S5.** <sup>1</sup>H NMR spectrum of the compound **1a**



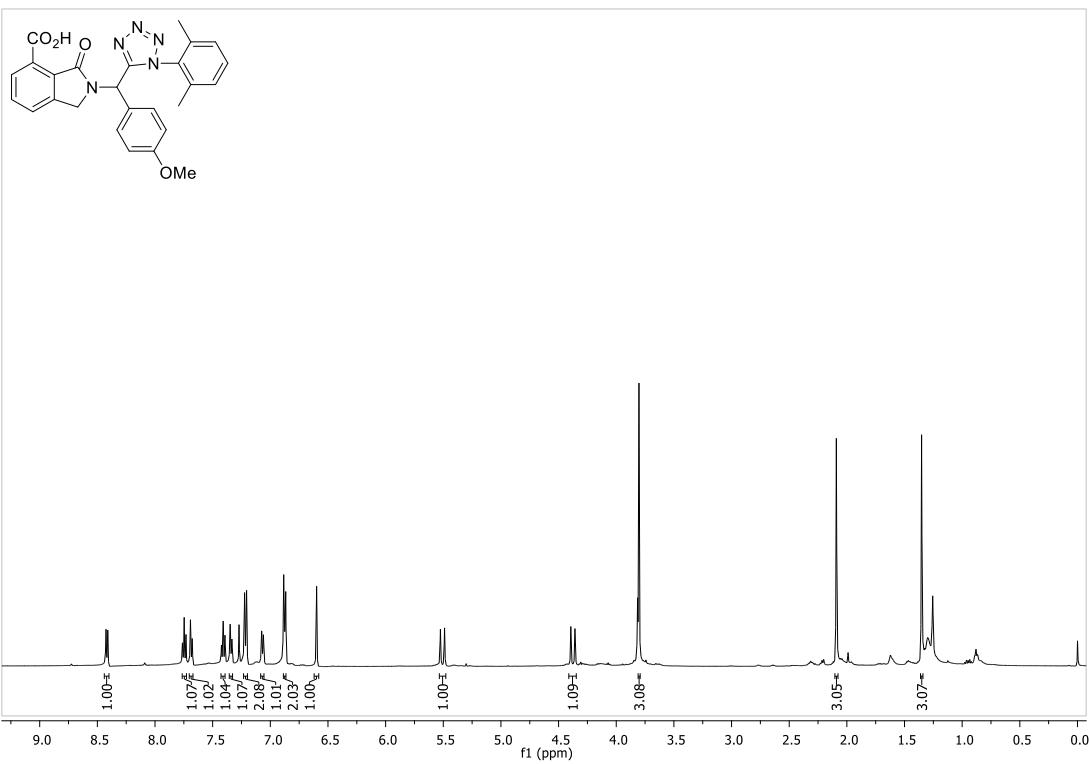
**Figure S6.** <sup>13</sup>C NMR spectrum of the compound **1a**



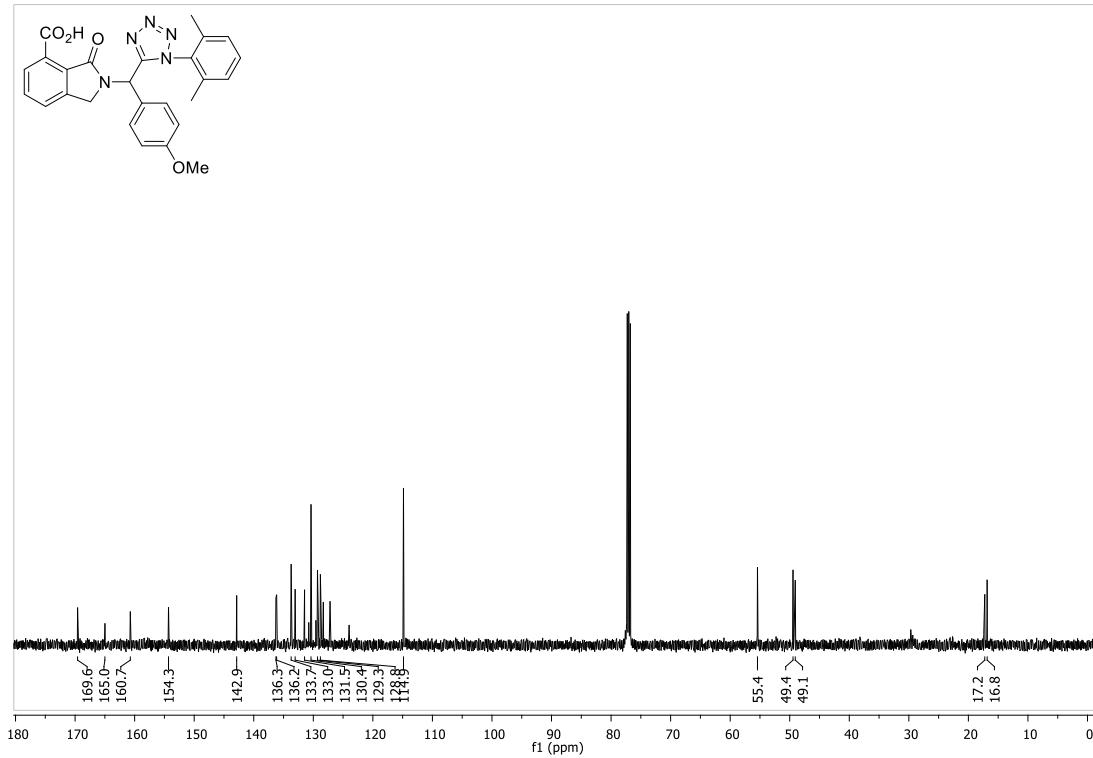
**Figure S7.**  $^1\text{H}$  NMR spectrum of the compound **1b**



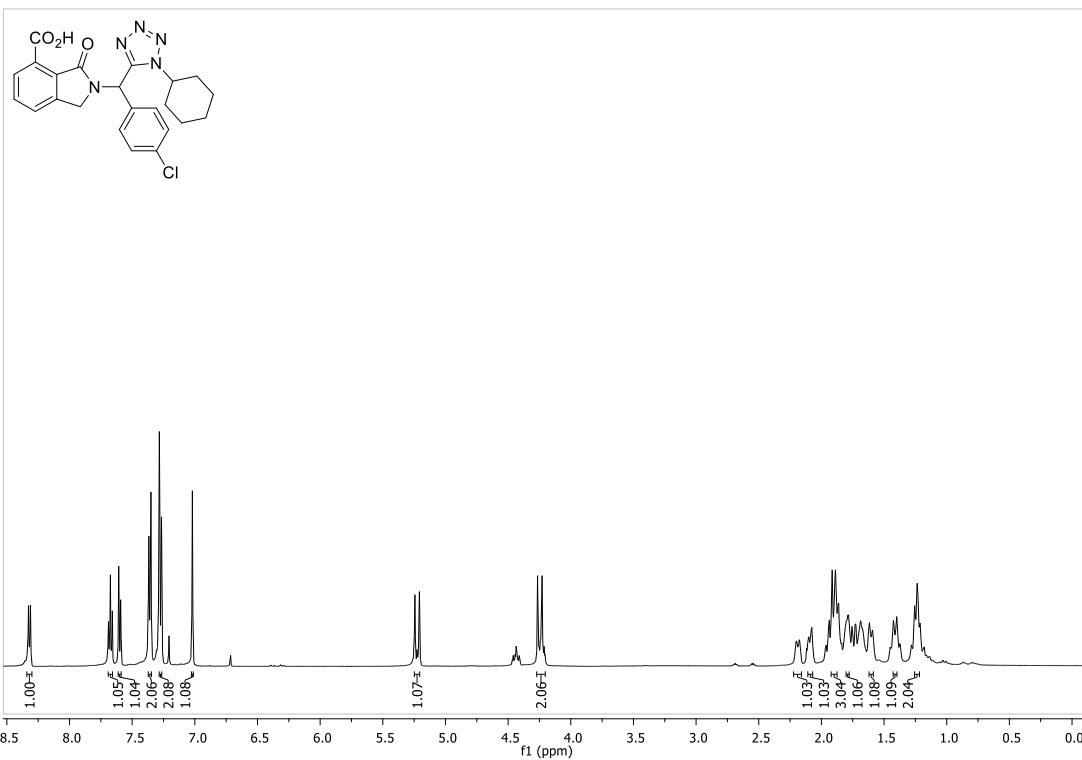
**Figure S8.**  $^{13}\text{C}$  NMR spectrum of the compound **1b**



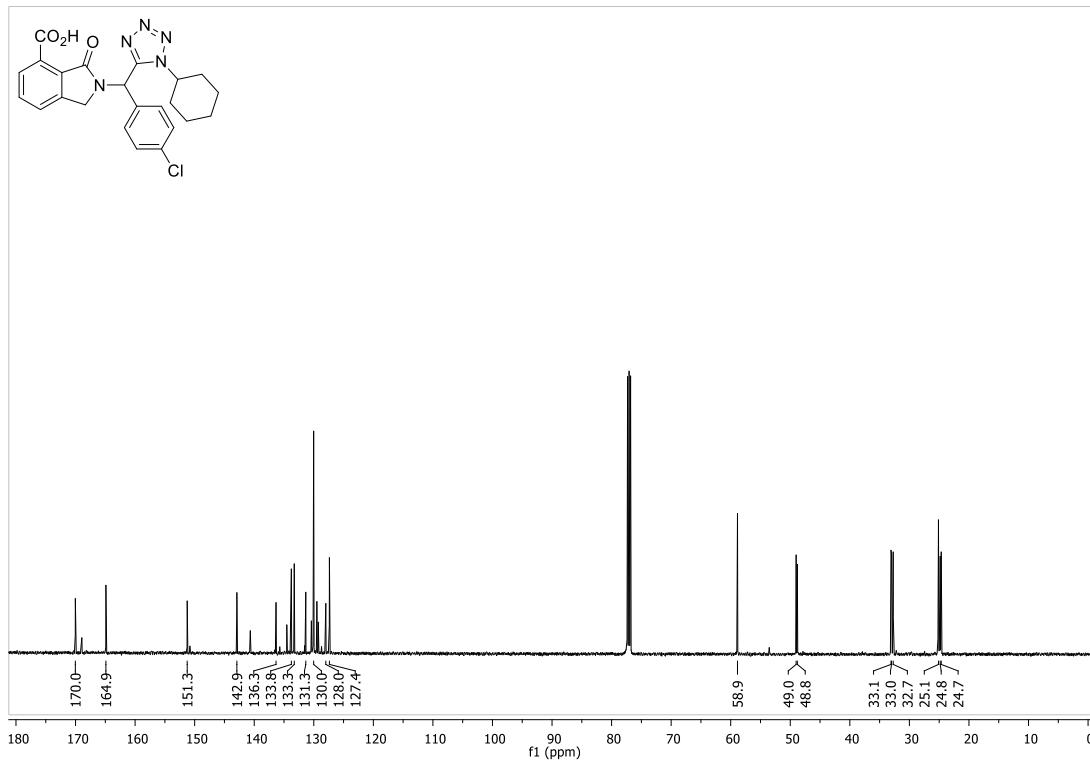
**Figure S9.**  $^1\text{H}$  NMR spectrum of the compound **1c**



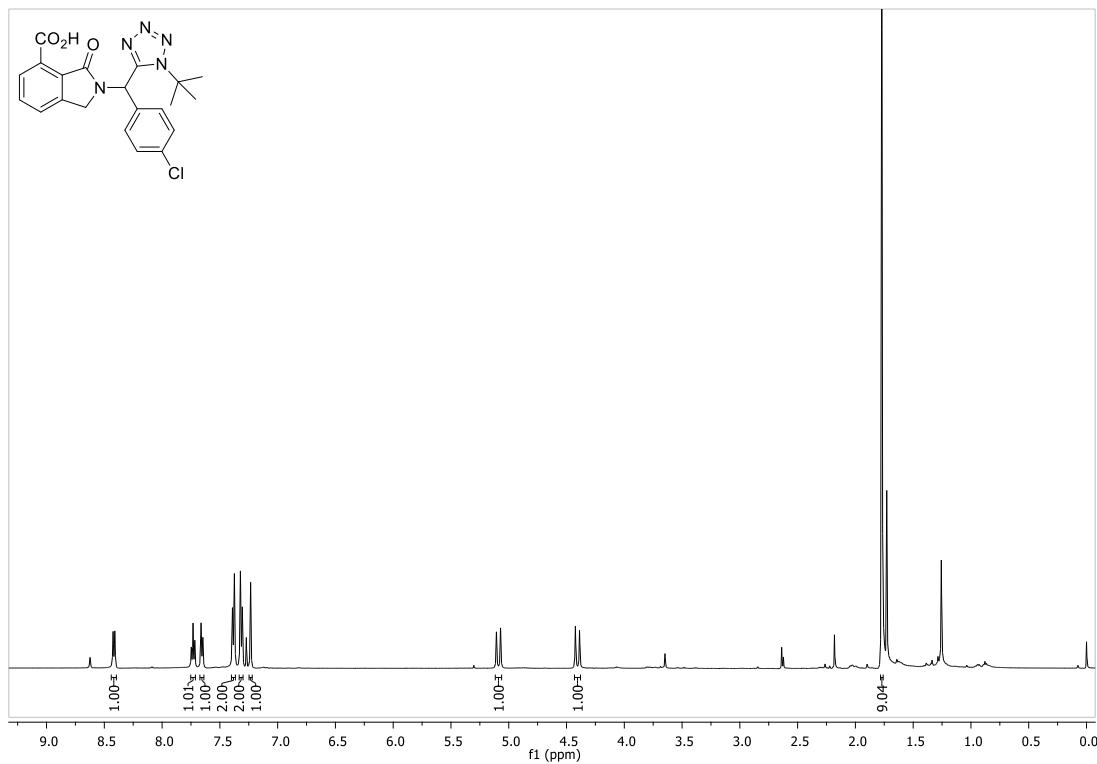
**Figure S10.**  $^{13}\text{C}$  NMR spectrum of the compound **1c**



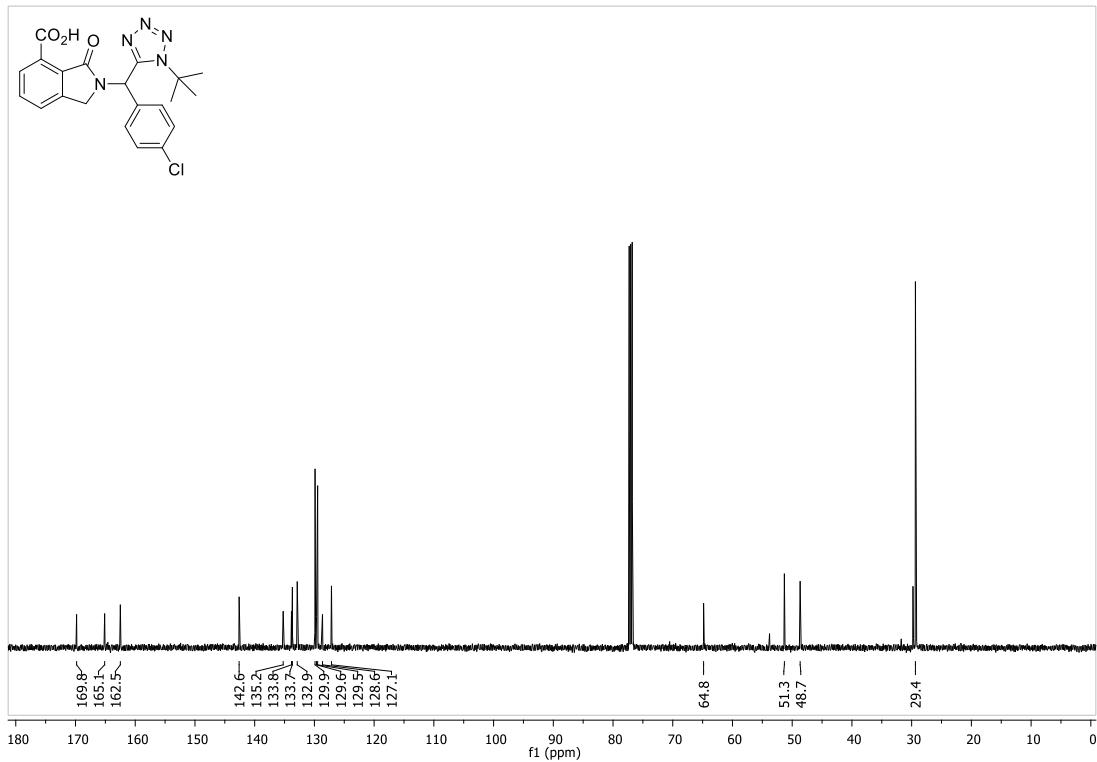
**Figure S11.** <sup>1</sup>H NMR spectrum of the compound **1d**



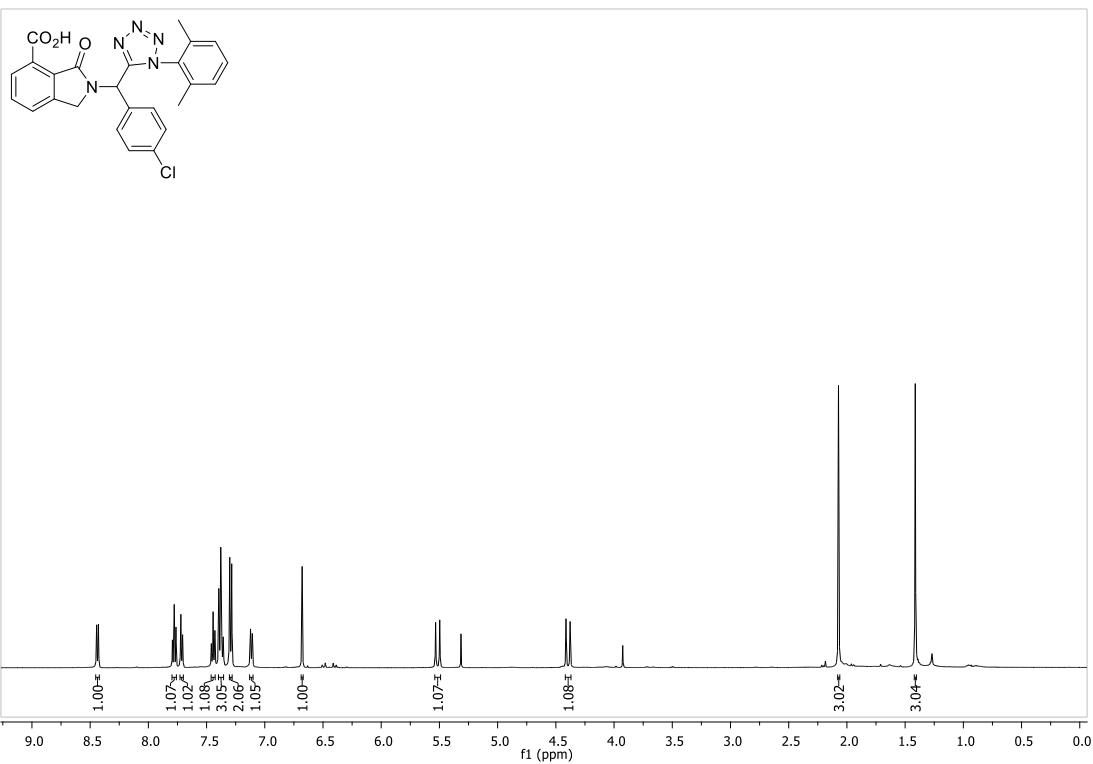
**Figure S12.** <sup>13</sup>C NMR spectrum of the compound **1d**



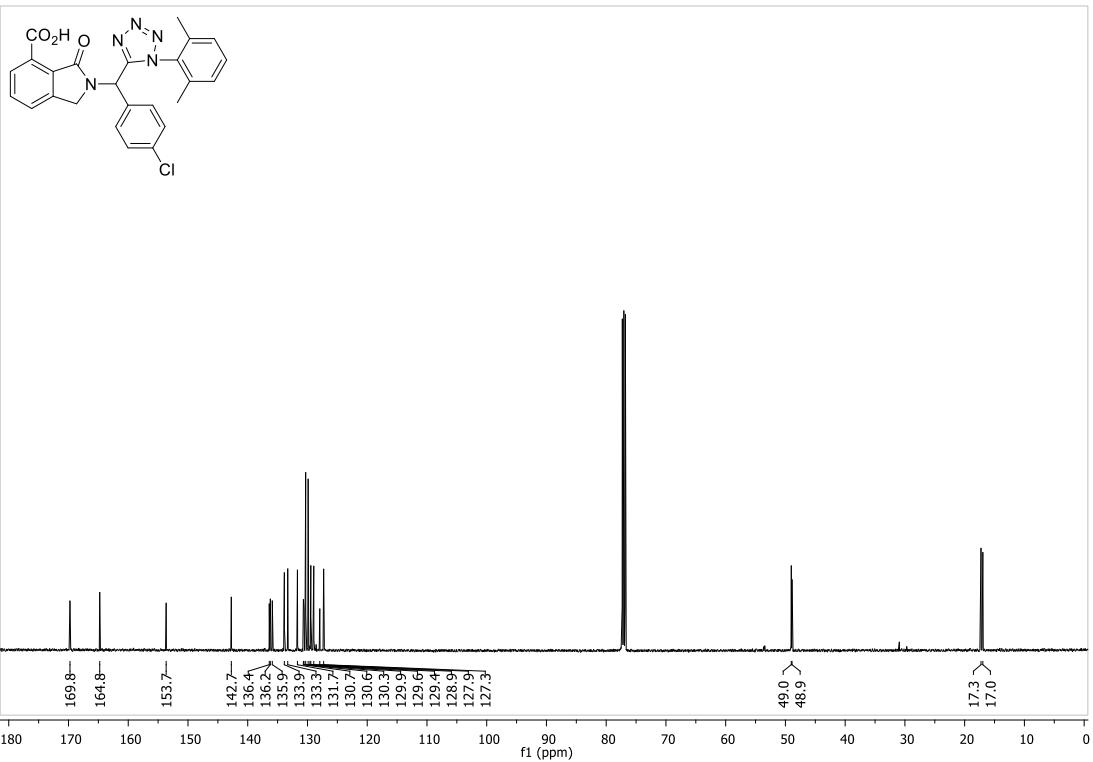
**Figure S13.**  $^1\text{H}$  NMR spectrum of the compound **1e**



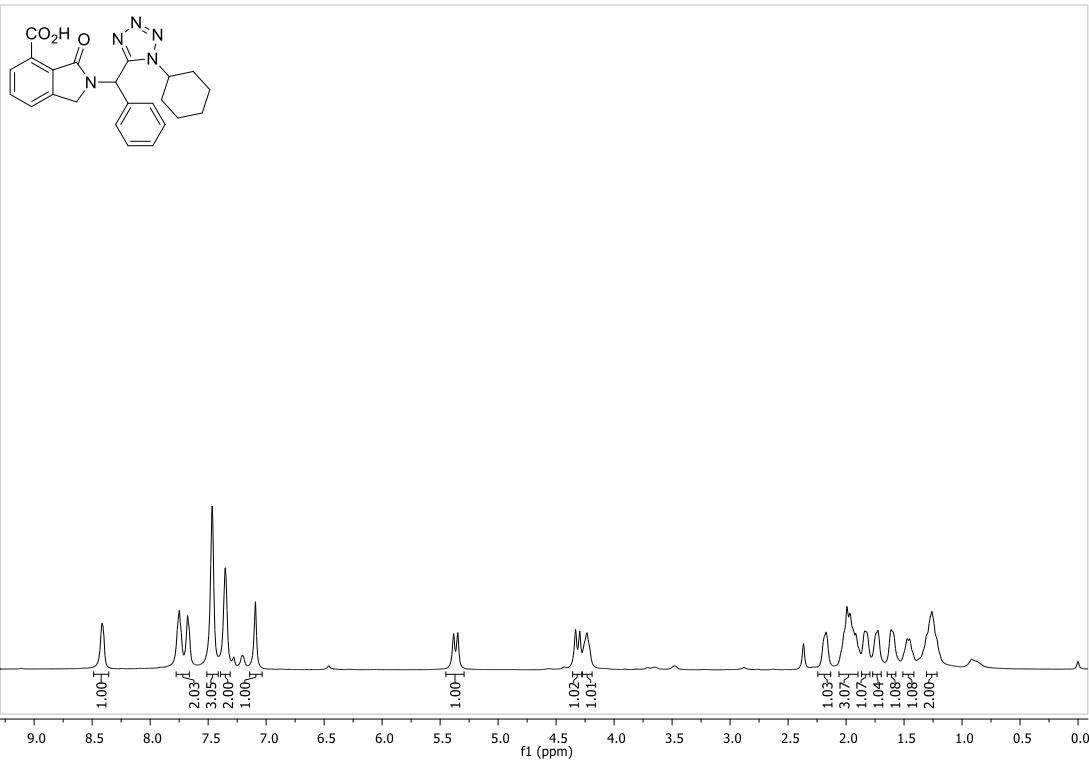
**Figure S14.**  $^{13}\text{C}$  NMR spectrum of the compound **1e**



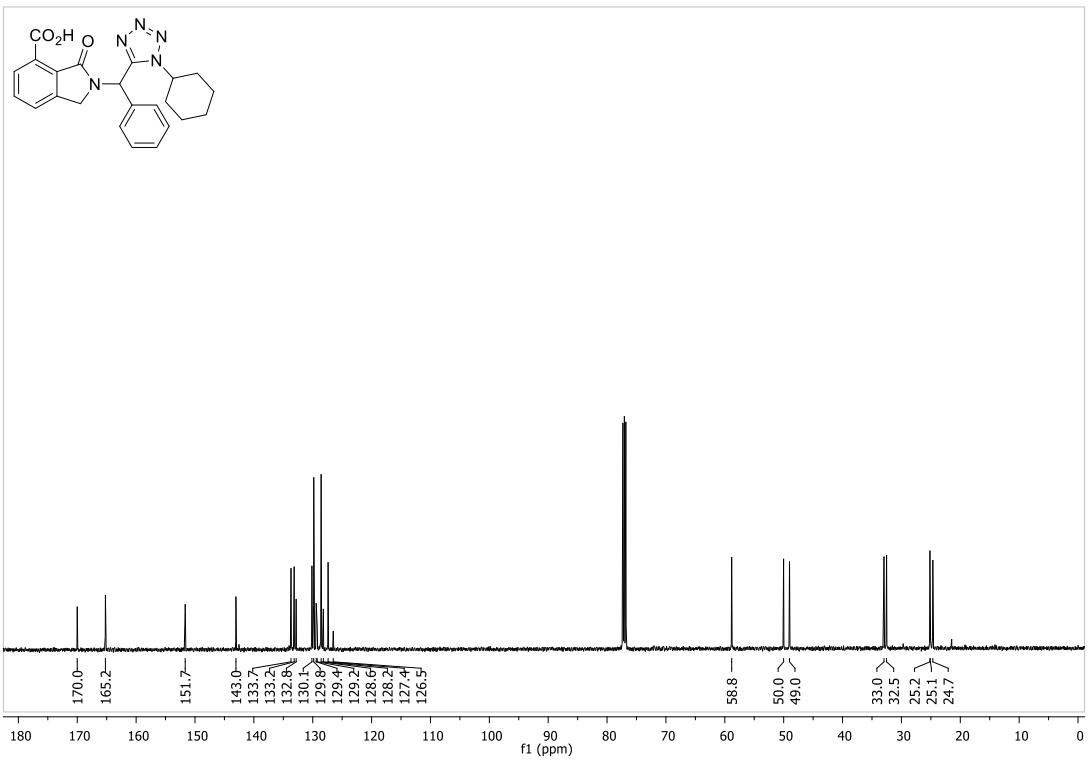
**Figure S15.** <sup>1</sup>H NMR spectrum of the compound **1f**



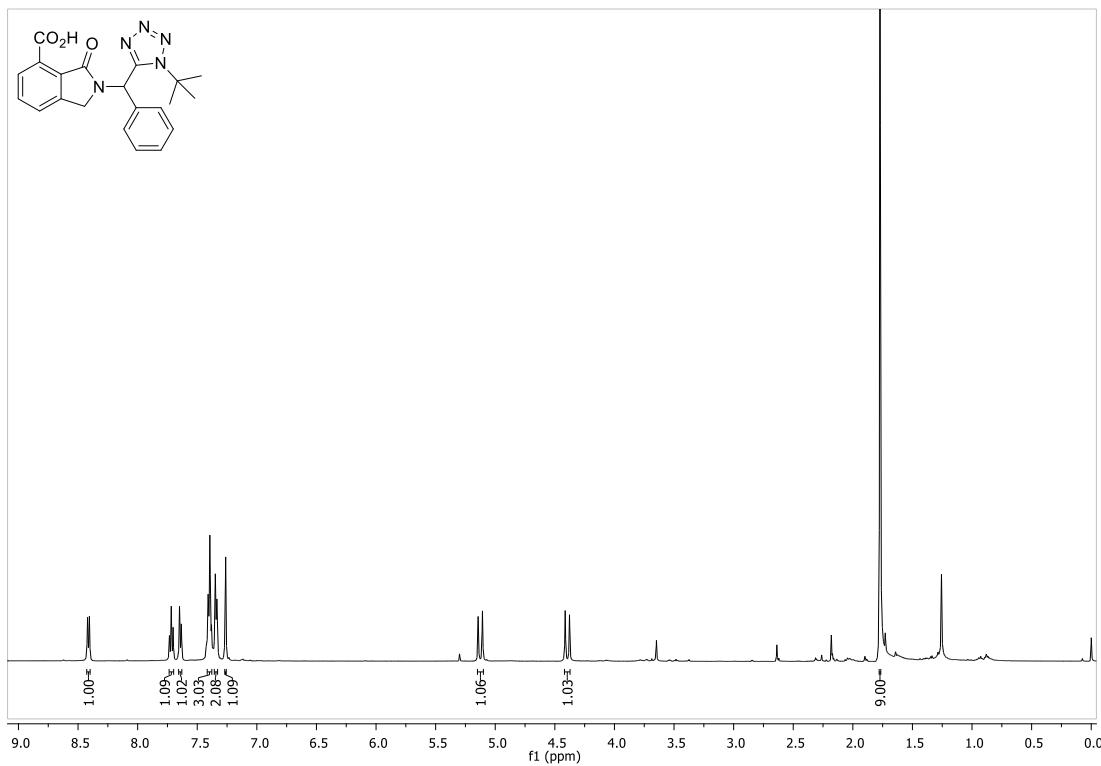
**Figure S16.** <sup>13</sup>C NMR spectrum of the compound **1f**



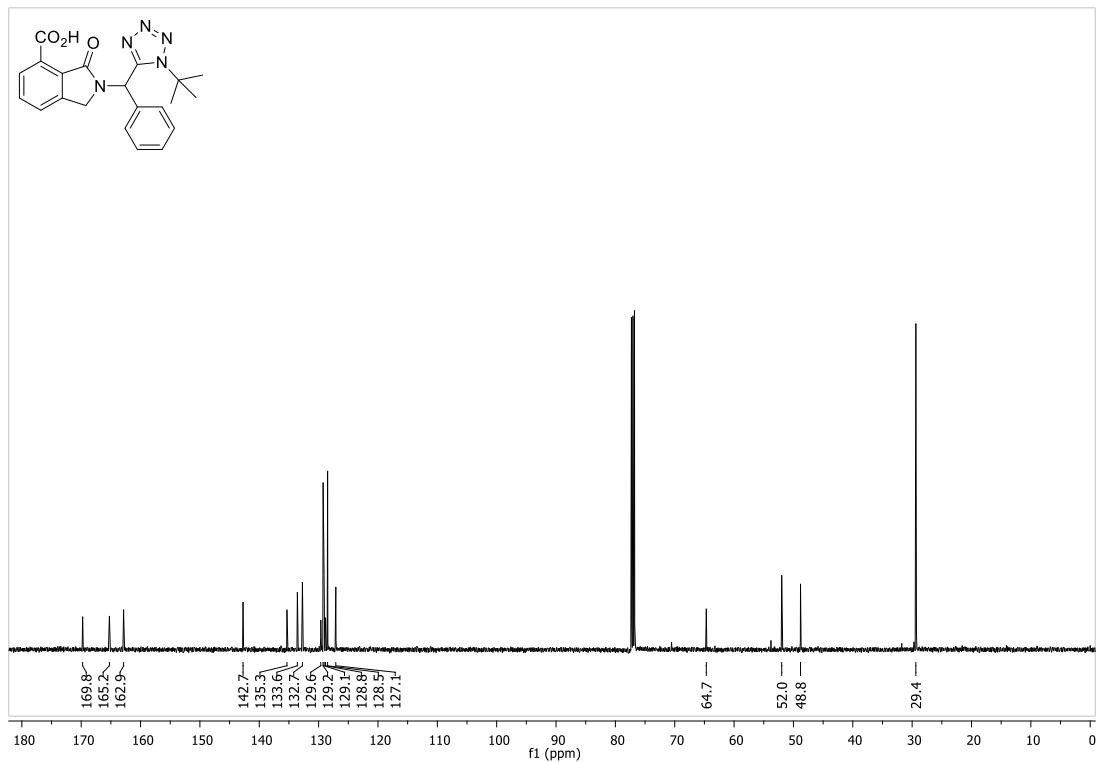
**Figure S17.**  $^1\text{H}$  NMR spectrum of the compound **1g**



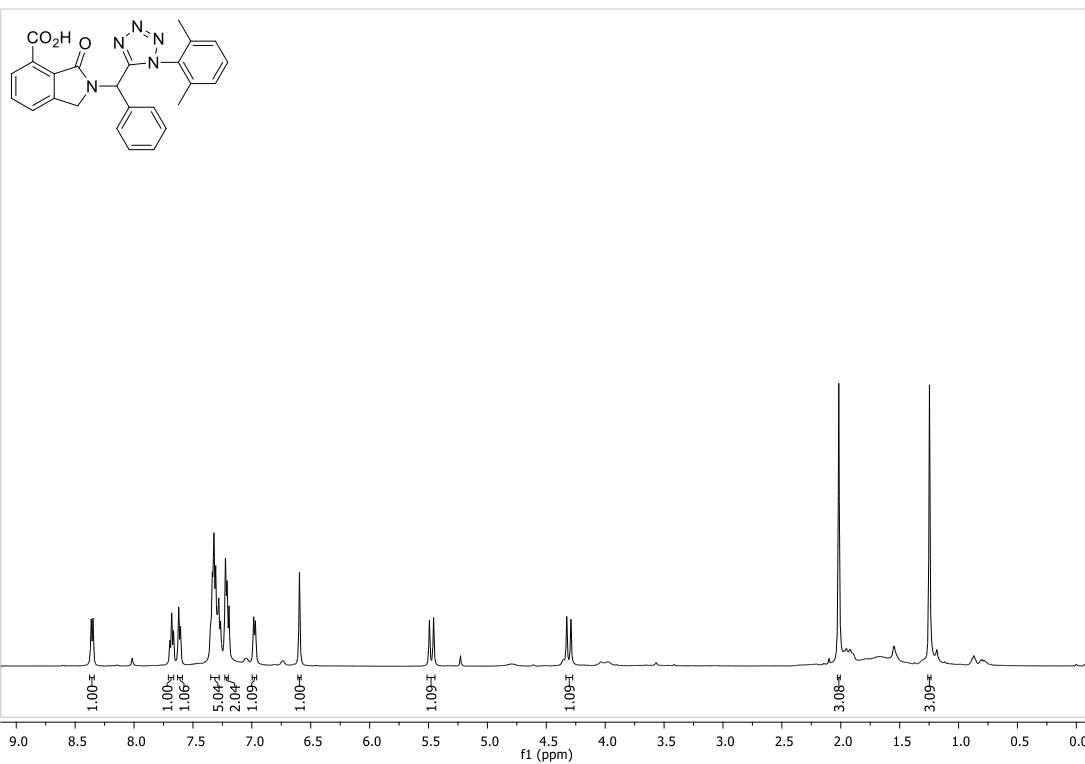
**Figure S18.**  $^{13}\text{C}$  NMR spectrum of the compound **1g**



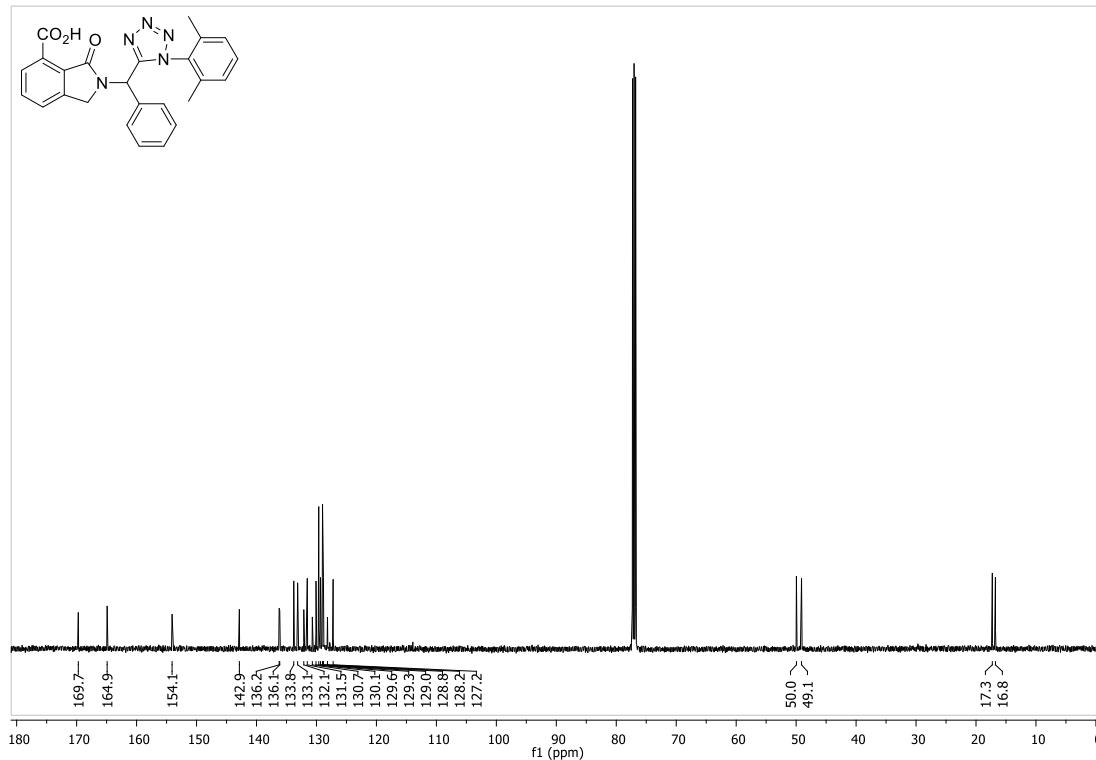
**Figure S19.**  $^1\text{H}$  NMR spectrum of the compound **1h**



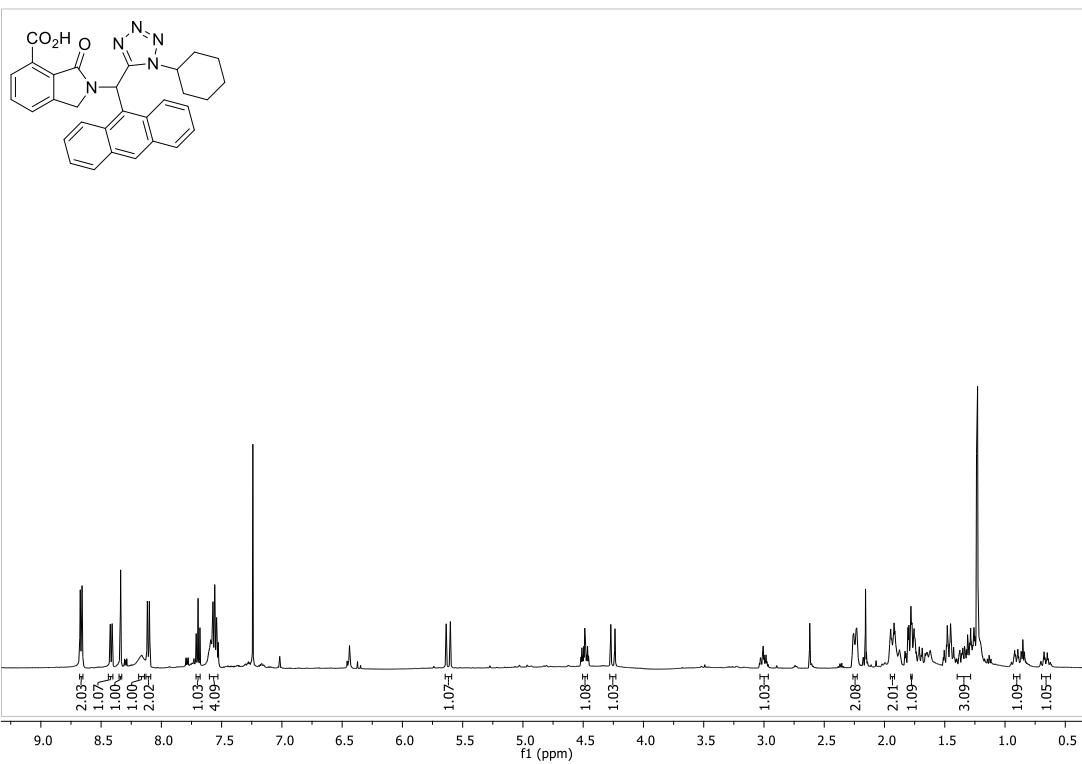
**Figure S20.**  $^{13}\text{C}$  NMR spectrum of the compound **1h**



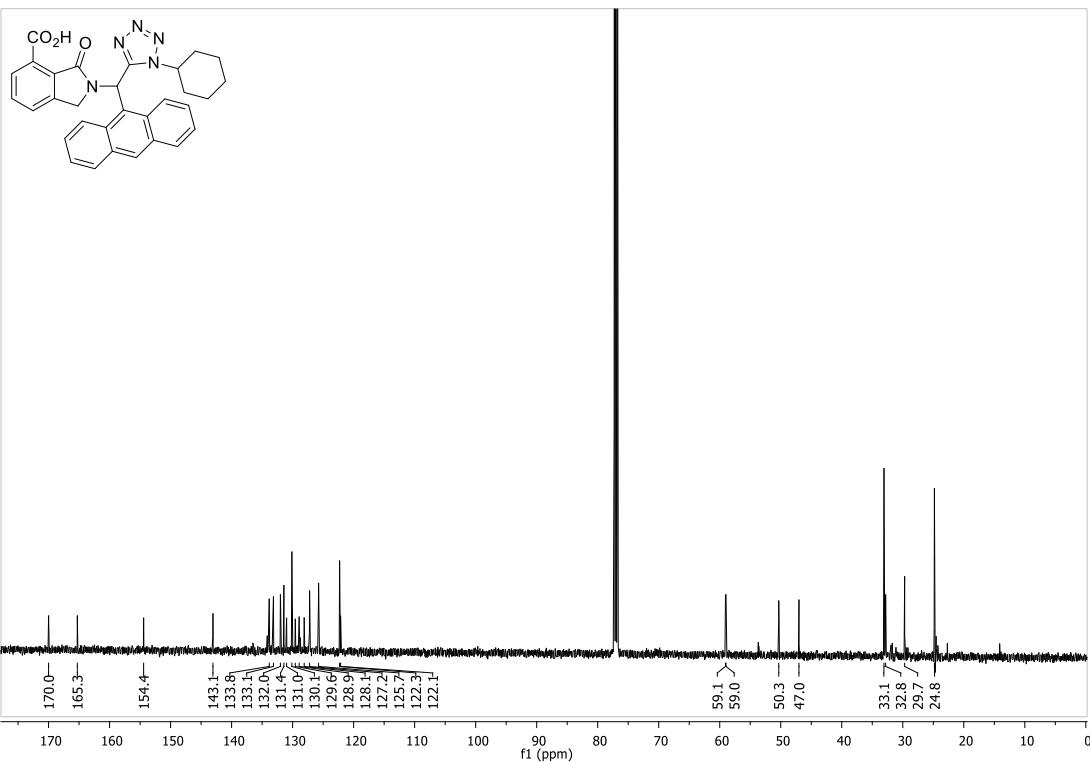
**Figure S21.** <sup>1</sup>H NMR spectrum of the compound **1i**



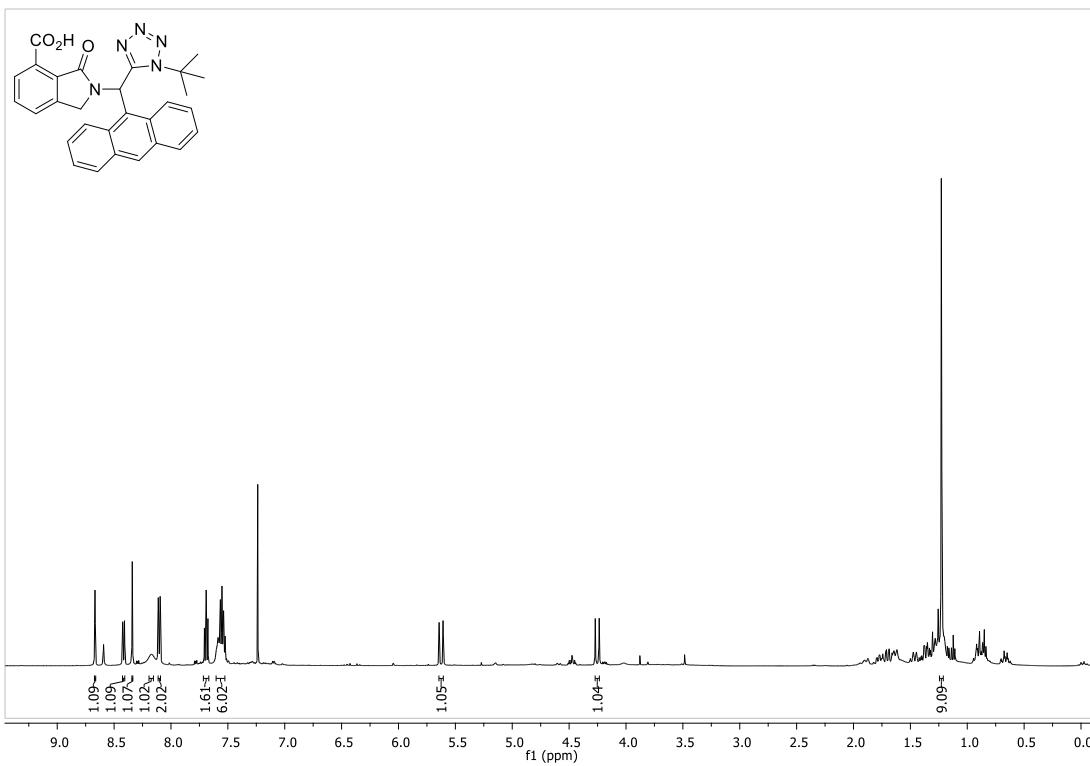
**Figure S22.** <sup>13</sup>C NMR spectrum of the compound **1i**



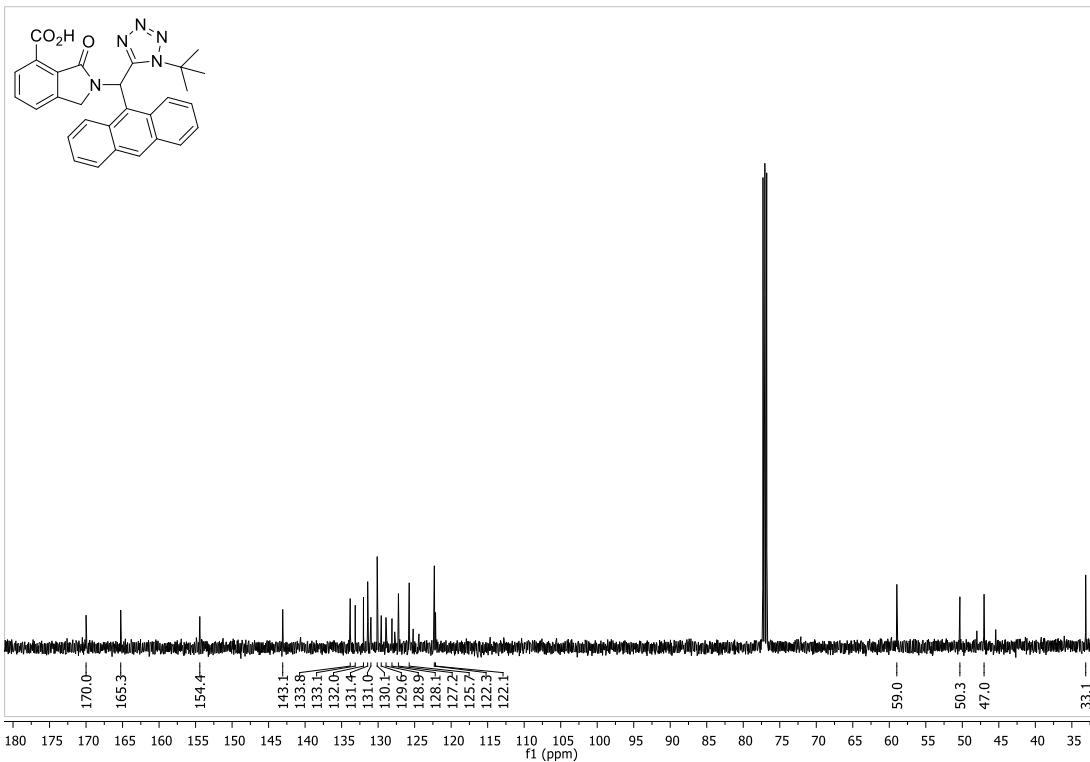
**Figure S23.** <sup>1</sup>H NMR spectrum of the compound **1j**



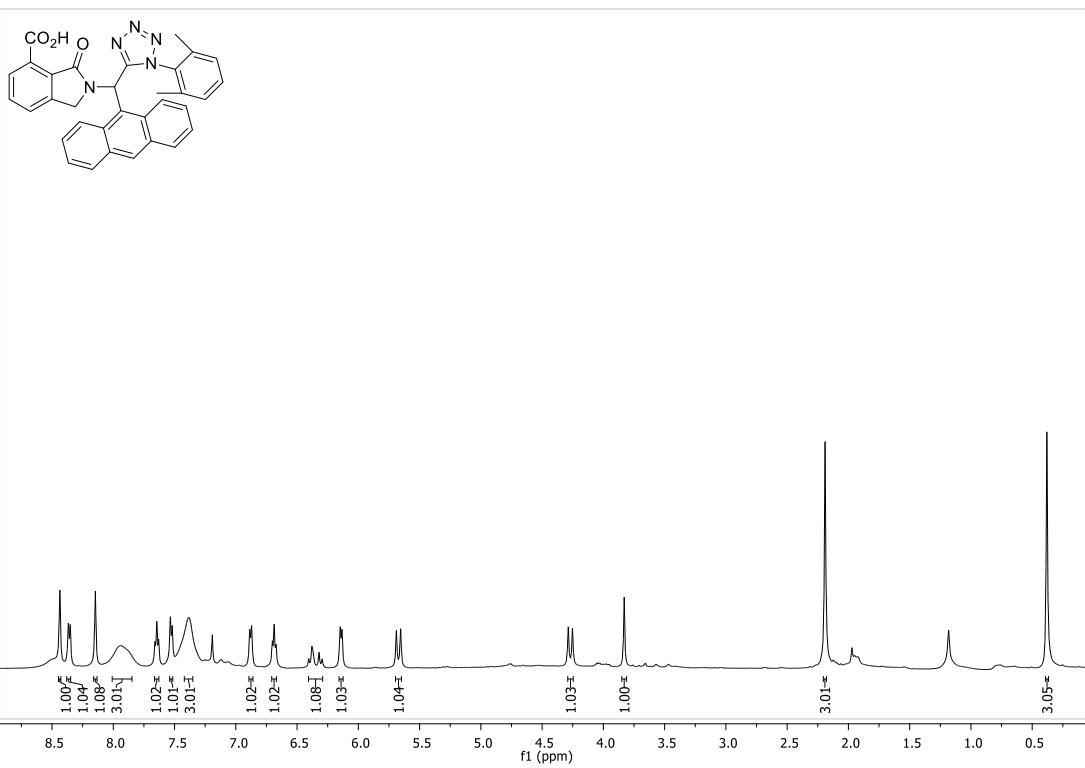
**Figure S24.** <sup>13</sup>C NMR spectrum of the compound **1j**



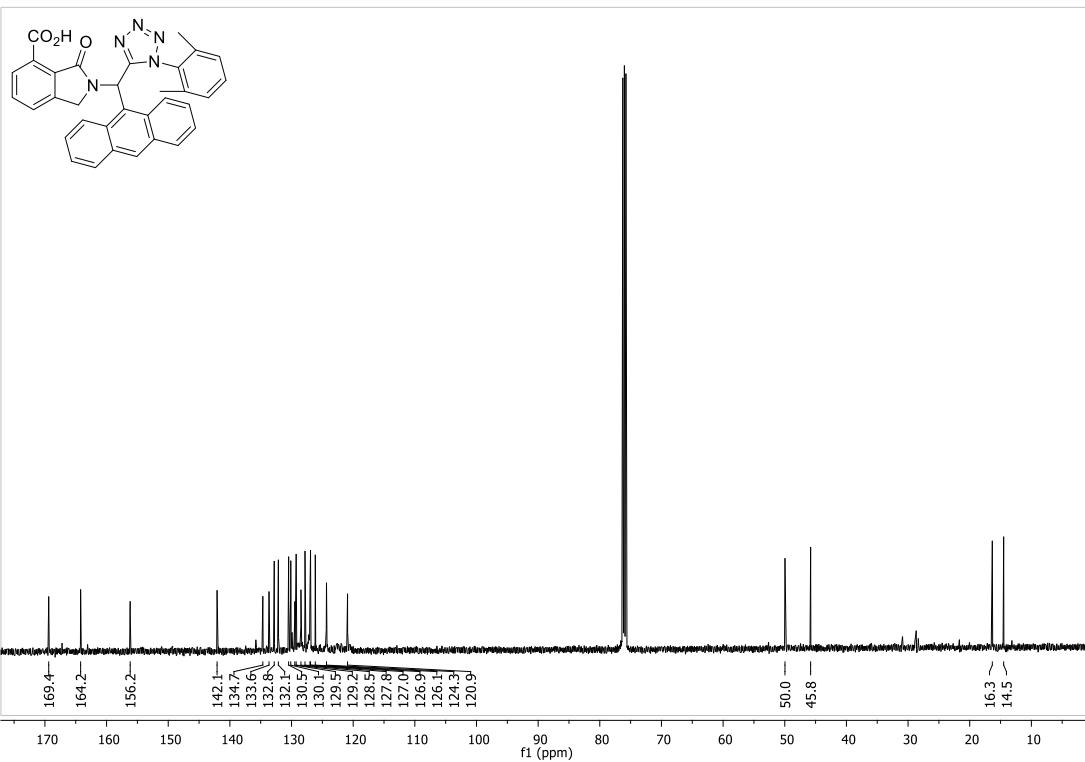
**Figure S25.**  $^1\text{H}$  NMR spectrum of the compound **1k**



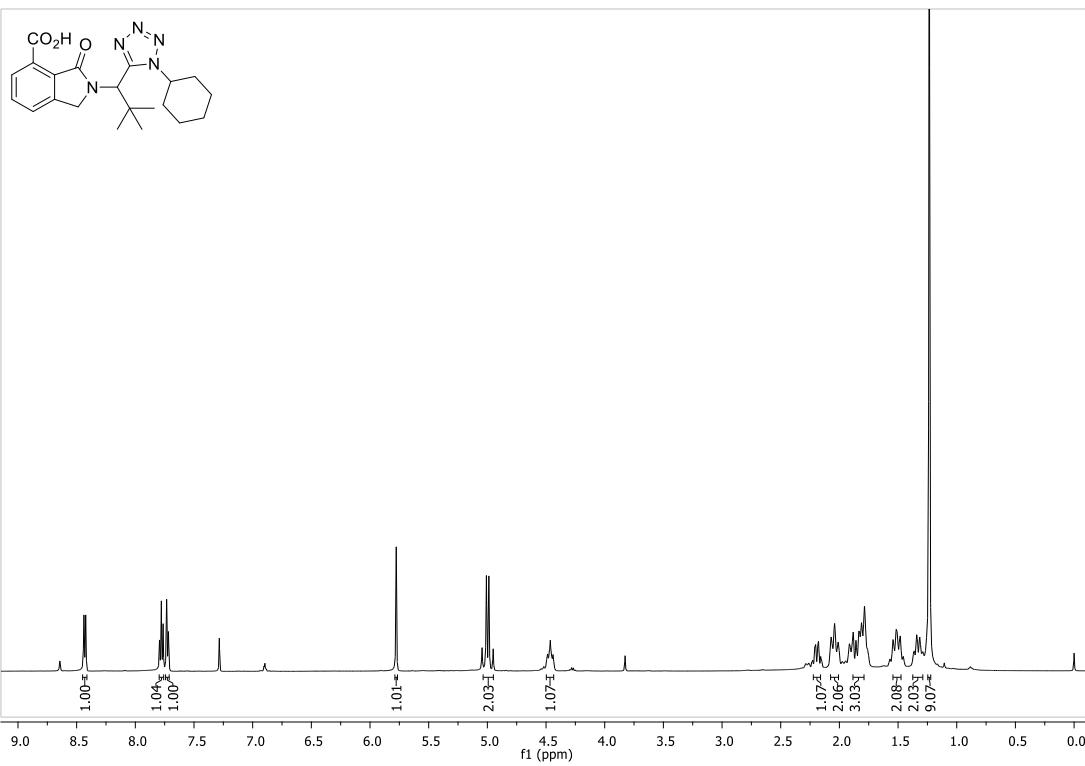
**Figure S26.**  $^{13}\text{C}$  NMR spectrum of the compound **1k**



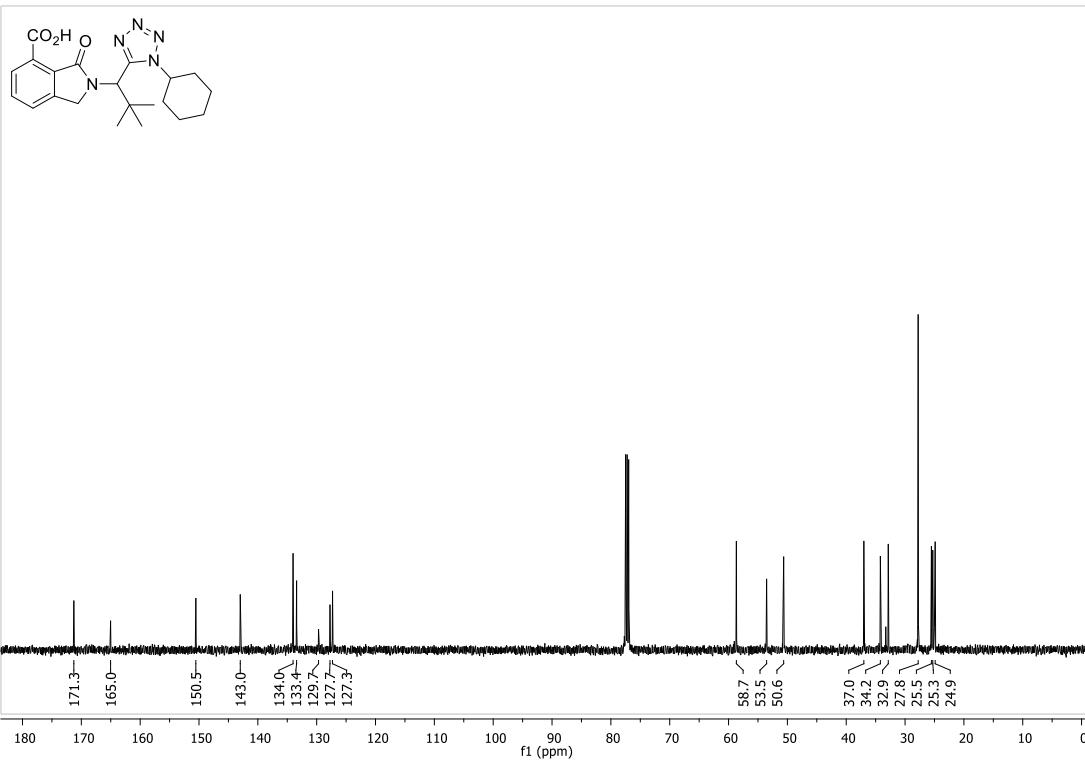
**Figure S27.**  $^1\text{H}$  NMR spectrum of the compound **11**



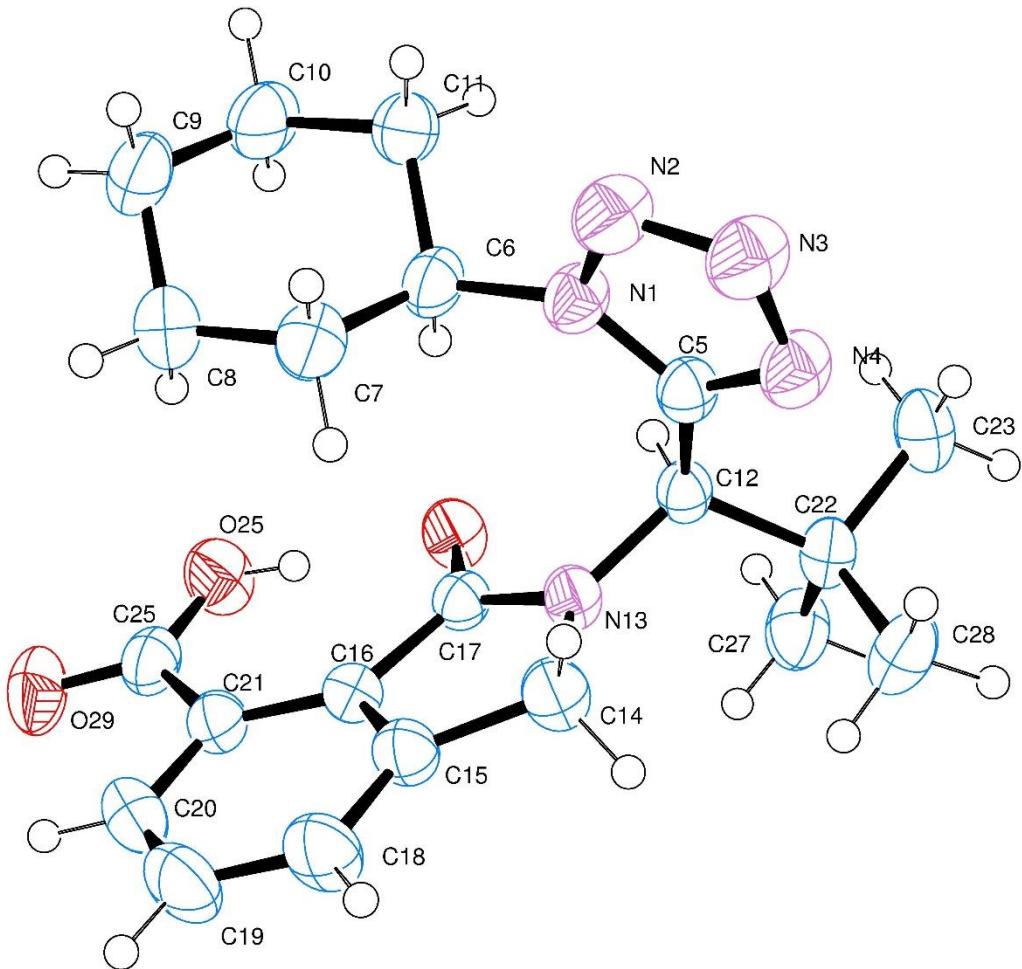
**Figure S28.**  $^{13}\text{C}$  NMR spectrum of the compound **11**



**Figure S29.**  $^1\text{H}$  NMR spectrum of the compound **1m**



**Figure S30.**  $^{13}\text{C}$  NMR spectrum of the compound **1m**



**Figure S31.** ORTEP of the product **1m**. Thermal ellipsoids were drawn at 50% probability level.

#### X-ray structure determination of the product **1m**

Single crystals of  $C_{21}H_{27}N_5O_3$  (**1m**) were obtained (Hexanes /  $CH_2Cl_2$  /  $CDCl_3$  = 80/10/10; v/v/v). Then, a suitable crystal was selected and mounted on a glass fiber using paraton N on a Xcalibur, Atlas, Gemini diffractometer. The crystal was kept at 291 K during data collection. Using Olex2,<sup>1</sup> the structure was solved with the ShelXS<sup>2</sup> structure solution program using direct methods and refined with the ShelXL<sup>3</sup> refinement package using Least Squares minimization.

## Refinement model description

Number of restraints – 0, number of constraints – unknown.

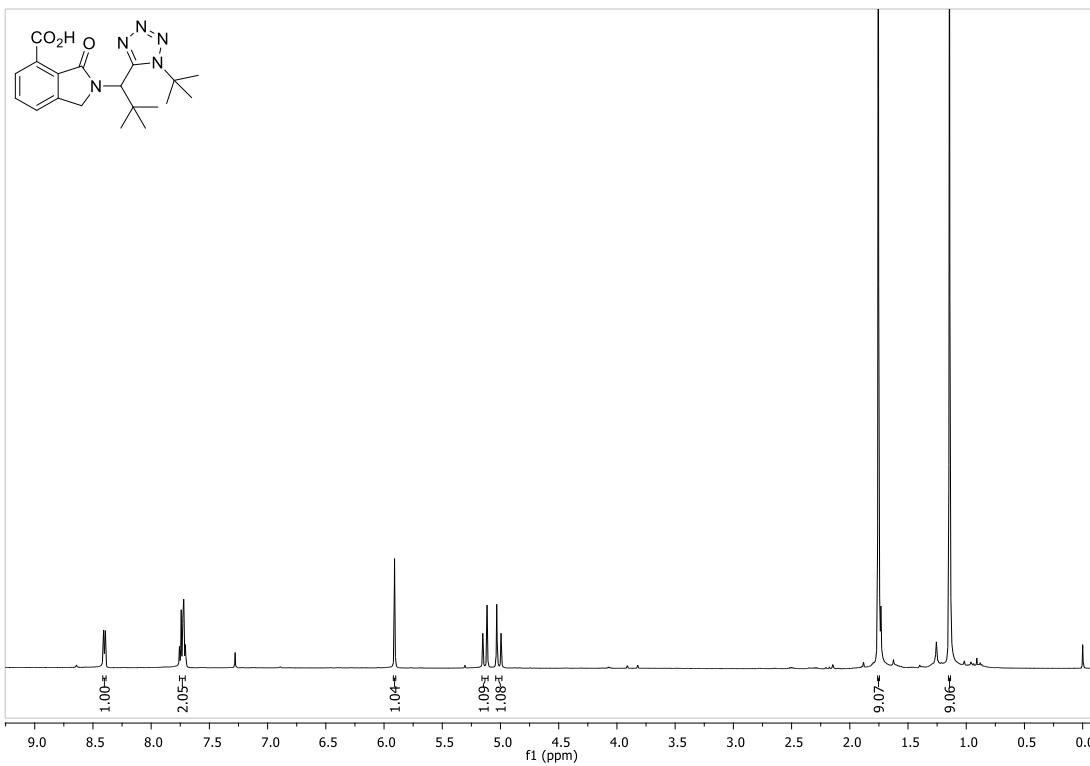
Details:

1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups At 1.5 times of: All C(H,H,H) groups, All O(H) groups
- 2.a Ternary CH refined with riding coordinates: C6(H6), C12(H12)
- 2.b Secondary CH<sub>2</sub> refined with riding coordinates: C7(H7A,H7B), C8(H8A,H8B), C9(H9A,H9B), C10(H10A,H10B), C11(H11A,H11B), C14(H14A,H14B)
- 2.c Aromatic/amide H refined with riding coordinates: C18(H18), C19(H19), C20(H20)
- 2.d Idealised Me refined as rotating group: C23(H23A,H23B,H23C), C27(H27A,H27B,H27C), C28(H28A,H28B,H28C)
- 2.e Idealized tetrahedral OH refined as rotating group: O25(H25)

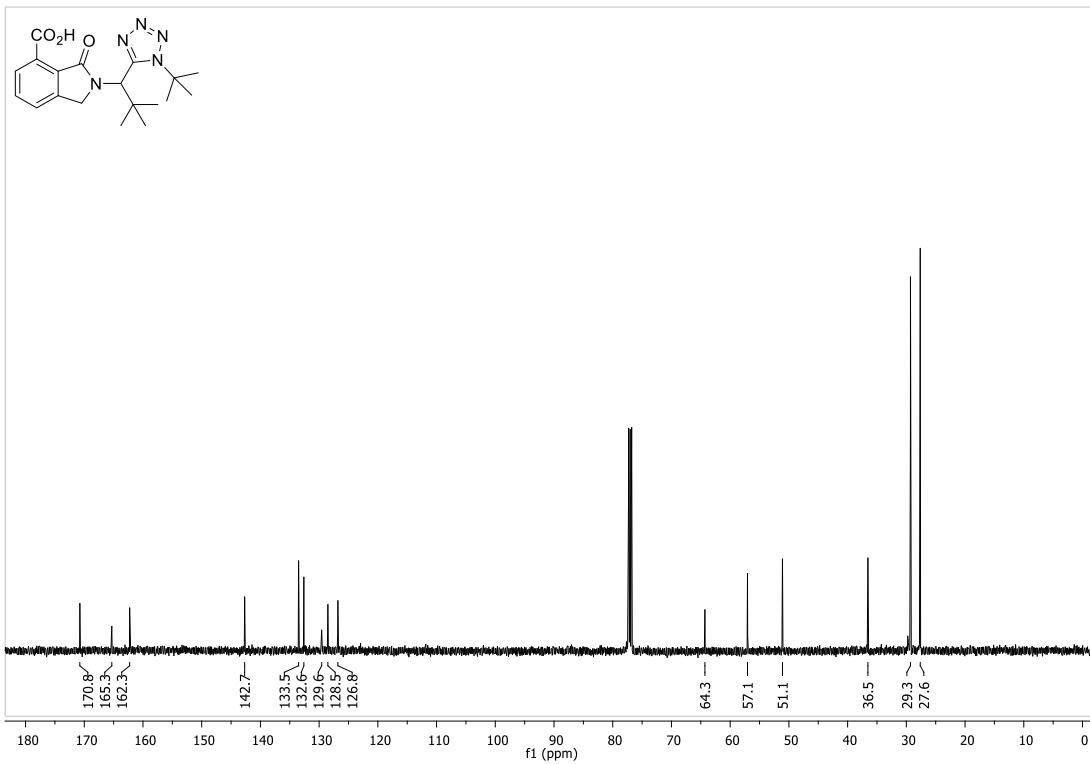
**Table S1.** Crystal data and structure refinement for compound **1m**

Identification code	srl268_JCMV50
Empirical formula	C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> O <sub>3</sub>
Formula weight	397.48
Temperature/K	291
Crystal system	triclinic
Space group	P-1
a/Å	9.2469(4)
b/Å	10.8452(5)
c/Å	11.8162(6)
α/°	102.960(4)
β/°	104.714(4)
γ/°	107.837(4)
Volume/Å <sup>3</sup>	1030.65(8)
Z	2
ρcalc (g/cm <sup>3</sup> )	1.281
μ/mm <sup>-1</sup>	0.715
F(000)	424.0
Crystal size/mm <sup>3</sup>	0.2 × 0. × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.19 to 155.02
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	21428
Independent reflections	4355 [R <sub>int</sub> = 0.0319, R <sub>sigma</sub> = 0.0209]
Data/restraints/parameters	4353/0/266
Goodness-of-fit on F2	1.038
Final R indexes [I>=2σ (I)]	R <sub>1</sub> = 0.0416, wR <sub>2</sub> = 0.1131
Final R indexes [all data]	R <sub>1</sub> = 0.0513, wR <sub>2</sub> = 0.1231
Largest diff. peak/hole / e Å <sup>-3</sup>	0.25/-0.19

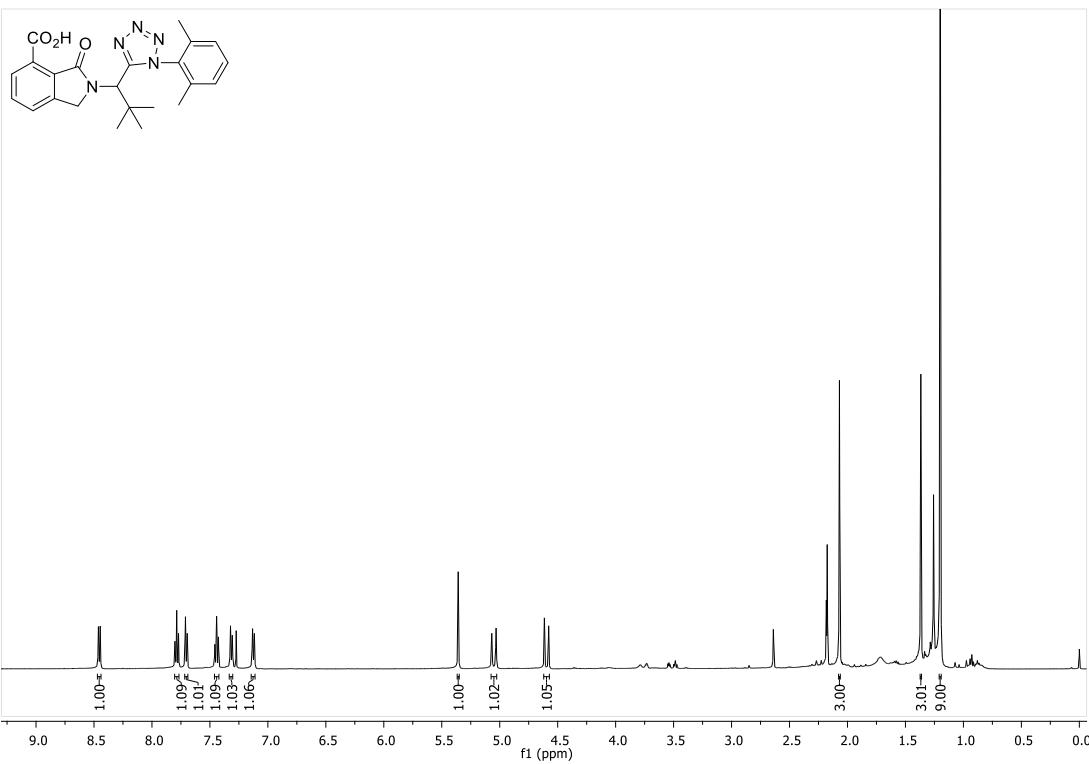
The crystallographic data for this structure was deposited in the Cambridge Crystallographic Data Centre (**CCDC-1503770**). Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK. ([deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)).



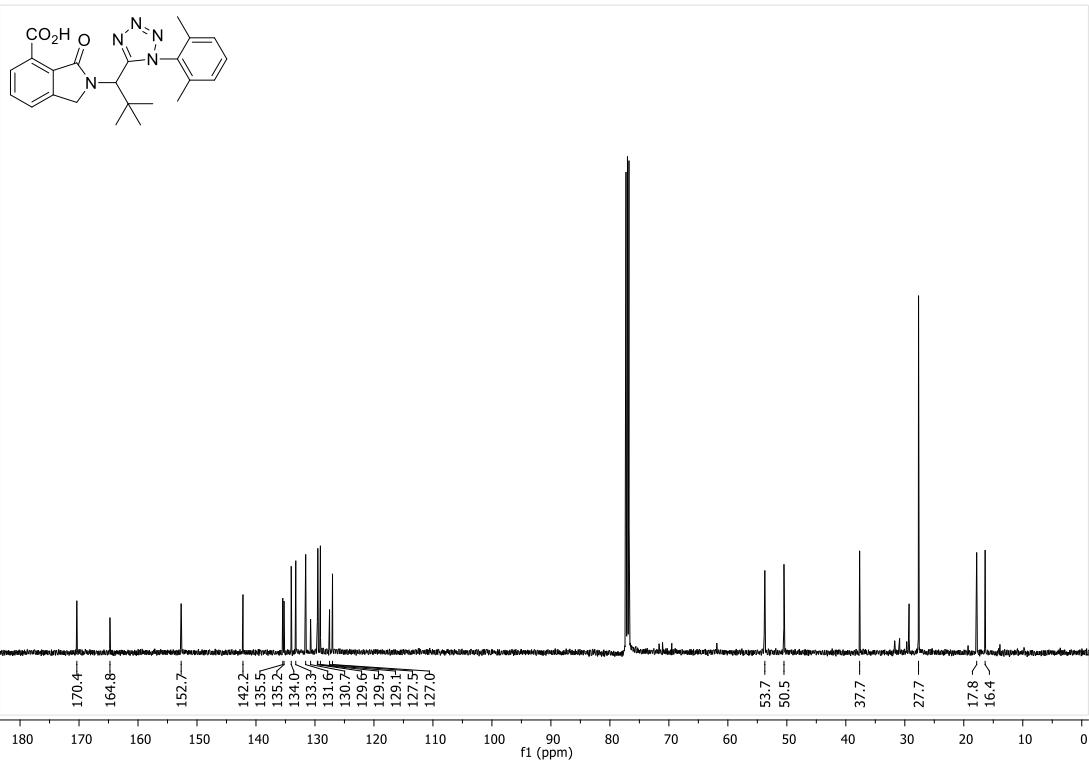
**Figure S32.**  $^1\text{H}$  NMR spectrum of the compound **1n**



**Figure S33.**  $^{13}\text{C}$  NMR spectrum of the compound **1n**



**Figure S34.** <sup>1</sup>H NMR spectrum of the compound **1o**



**Figure S35.** <sup>13</sup>C NMR spectrum of the compound **1o**

## COMPUTATIONAL STUDY

### COMPUTATIONAL DETAILS.

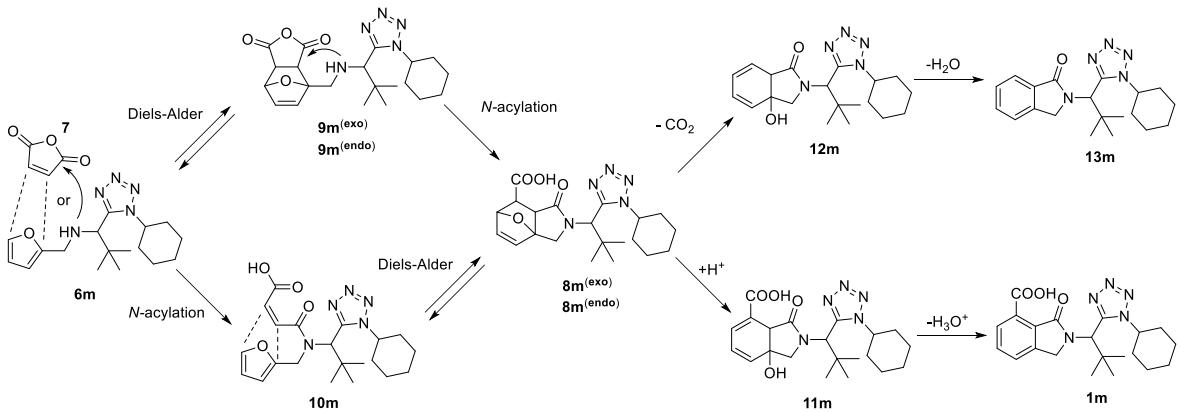
All of the DFT calculations were done using Gaussian09 package.<sup>4</sup> We first performed gas-phase geometry optimizations with the hybrid *meta* exchange-correlation density-functional M06-2X<sup>5</sup> in combination with Pople's 6-31G(d) double- $\xi$  quality basis set with one polarization function in all atoms. A subsequent harmonic frequency calculation (for each optimized geometry) was executed to corroborate the character of each critical point in the potential energy surface (PES): reactants, products, intermediates and adducts must present all the frequencies as positive (eigenvalues of the Hessian matrix should be real) whereas transition states are characterized by one and only one negative frequency (one eigenvalue should be imaginary) which is commonly associated to the reaction coordinate in practical terms. These frequency calculations also allow us to compute the zero-point energy (ZPE) and thermal terms for expressing values as Gibbs free energies at 298K. Later, for improving the numerical precision in our reported self-consistent field (SCF) energies, we did single-point calculations over each optimized geometry using the same density-functional but this time using a triple- $\xi$  quality basis set: 6-311+G(d).

It is worth to note that we performed intrinsic reaction coordinate (IRC) calculations for each found transition state to follow the reaction coordinate downhill. Later, we also carried out consecutive geometry optimizations for both sides where IRC calculations came to a supposed minimum. This way, we ensured our transition states really connected both desired reactants and products in each reaction step.

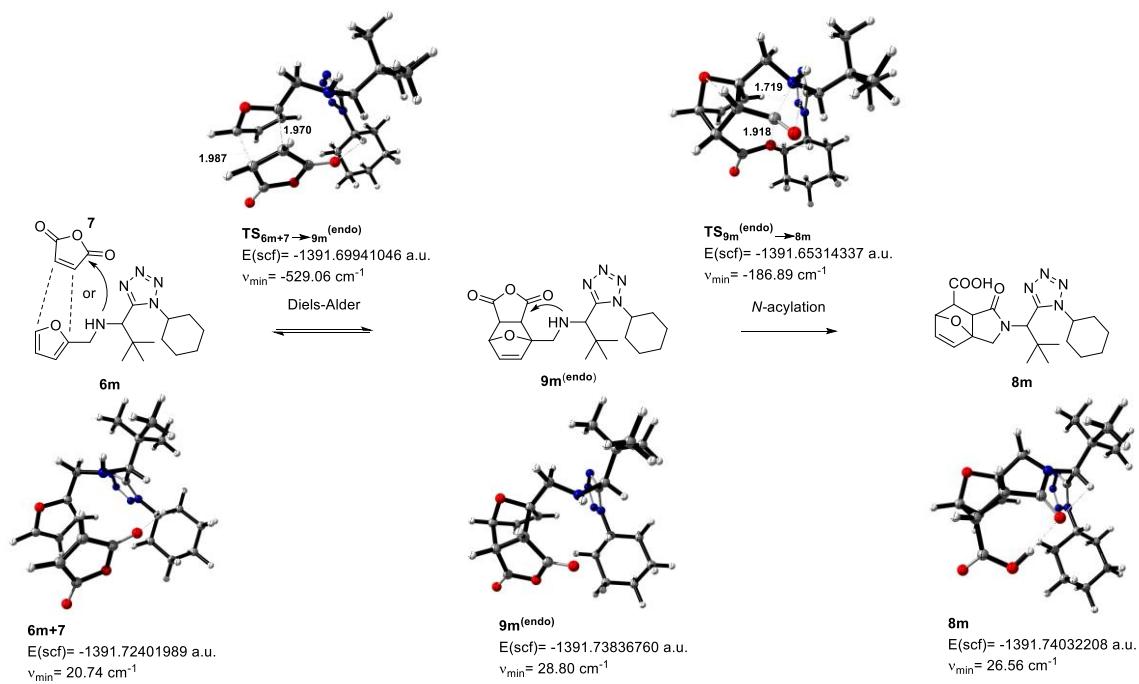
Finally, we have also considered solvation effects added to the electronic Hamiltonian by performing single-point calculations over the optimized geometries again but using the continuous polarizable conductor-like model (PCM)<sup>6</sup> with the UAKS atomic radii and the dielectric standard values for toluene, in concordance with our experimental findings.

Finally, we also have added dispersion corrections by means of the DFT-D3 method of Grimme (using the parameters for M06-2X density-functional:  $s^6 = 1.0000$ ,  $s^8 = 0.0000$ ,  $rs^6 = 1.6190$  and  $rs^{18} = 1.000$ ).<sup>7</sup>

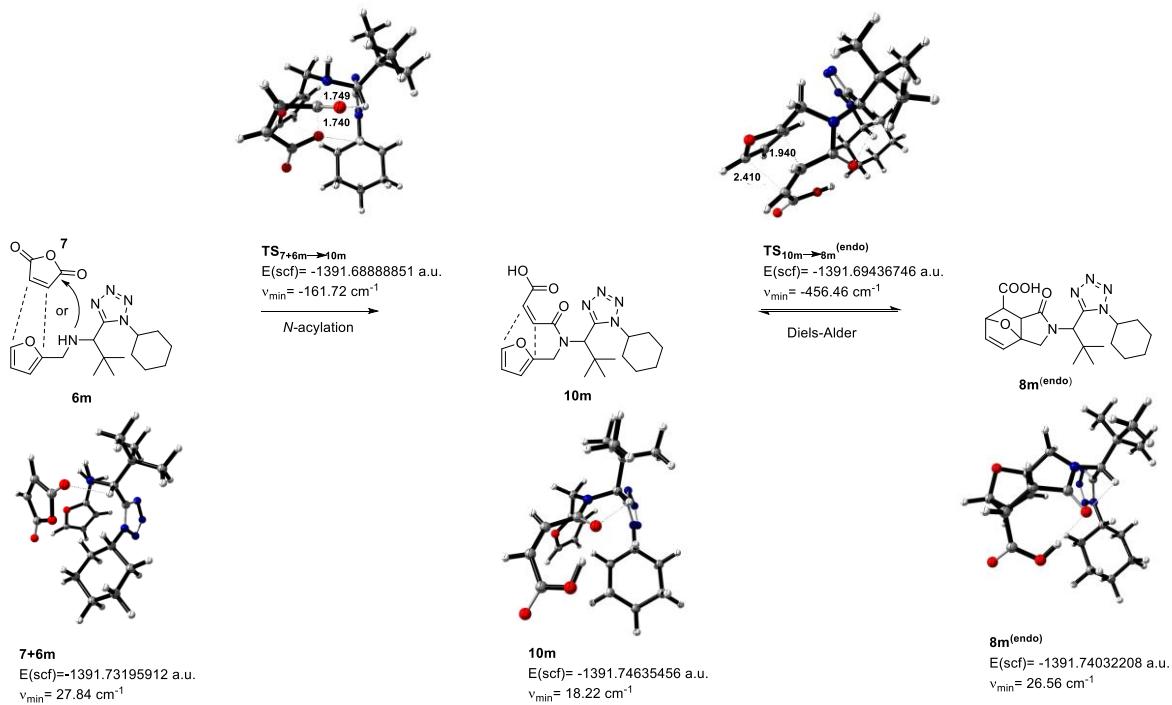
Therefore, our final reported energy values are in solvent-phase and the level of theory becomes PCM[M06-2X/6-311+G(d)//M06-2X-D3/6-31G(d)].



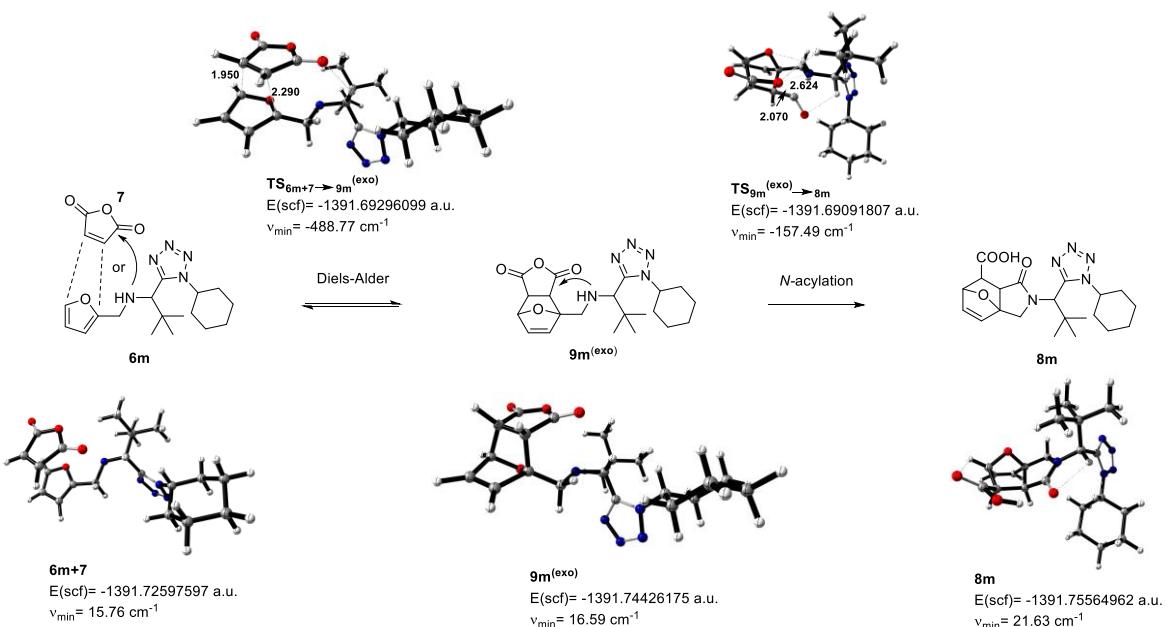
**Scheme S1.** Overview of the proposed reaction mechanism.



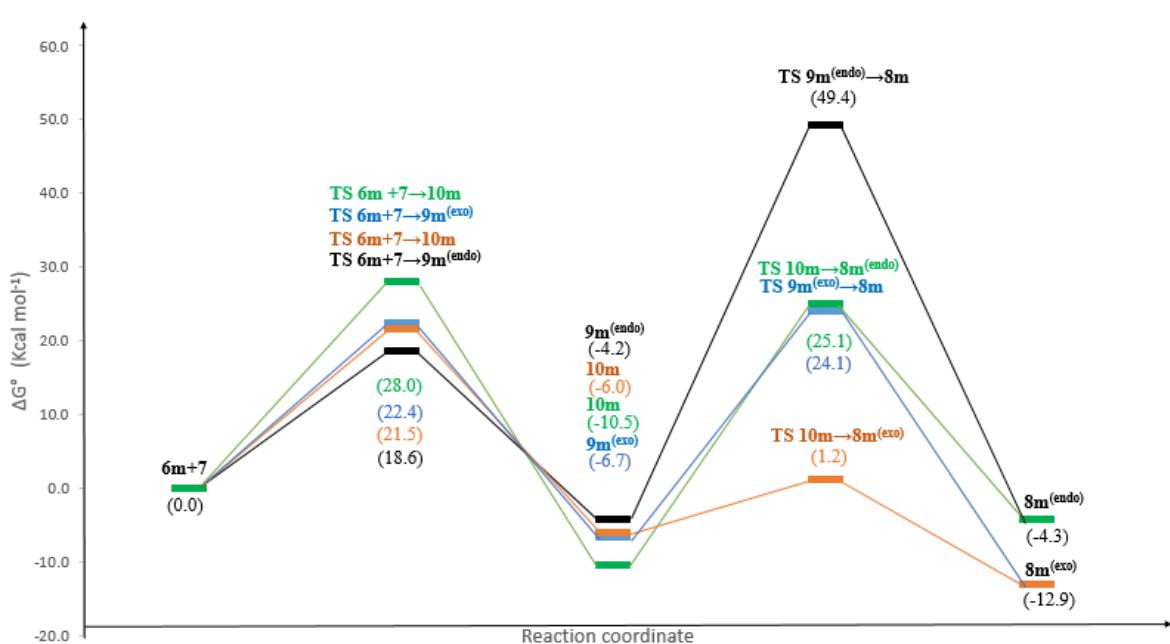
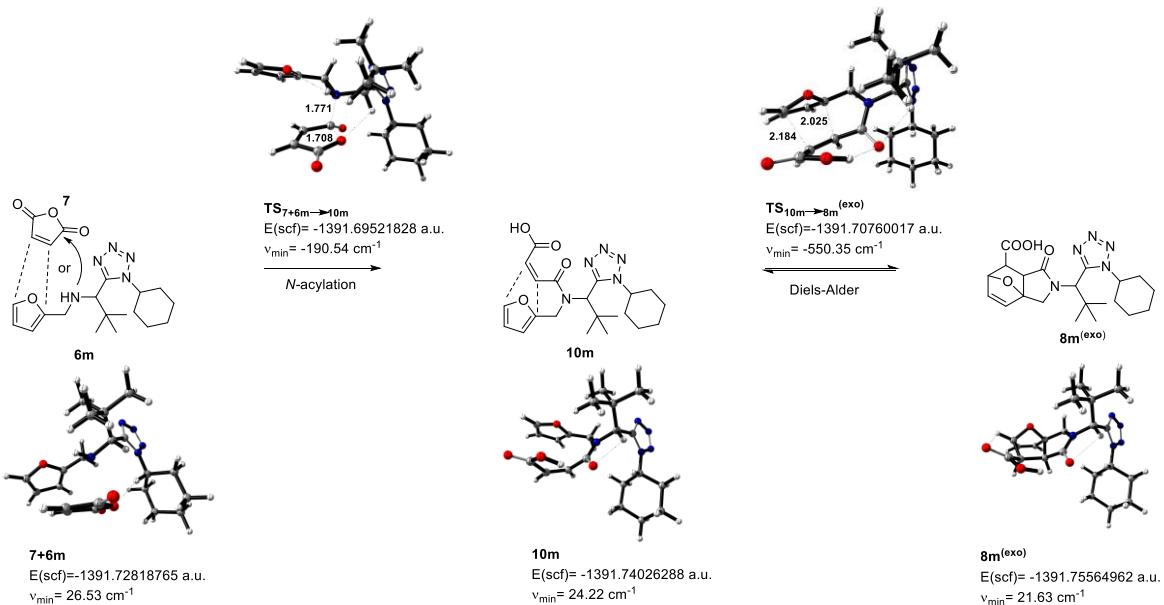
**Scheme S2.** Reaction path:  $\mathbf{6m} + \mathbf{7} \rightarrow \mathbf{9m}^{\text{(endo)}} \rightarrow \mathbf{8m}$ .



**Scheme S3.** Reaction path:  $6\mathbf{m} + \mathbf{7} \rightarrow \mathbf{10}\mathbf{m} \rightarrow \mathbf{8}\mathbf{m}^{(\text{endo})}$ .



**Scheme S4.** Reaction path:  $6\mathbf{m} + \mathbf{7} \rightarrow \mathbf{9}\mathbf{m}^{(\text{exo})} \rightarrow \mathbf{8}\mathbf{m}$ .



**Figure S36.** Energy profile for the whole route **6m** + **7** → **8m**.

The B3LYP hybrid density functional has a high popularity, but there have been alarming reports concerning large errors in energetics.<sup>8–11</sup> Zhao and Truhlar recommended the M06-2X functionals for main-group thermochemistry and kinetics.<sup>12–14</sup> M06-2X capture stacking effects,<sup>15</sup> which can be present in transition

states (TS). Besides, it has been shown that M06-2X is among the best methods for predicting reaction enthalpies and activation barriers for cycloaddition reactions.<sup>8, 16-17</sup>

To determine the reaction mechanism, DFT calculations were performed using the robust method PCM(Toluene)[M06-2X/6-311+G(d)//M06-2X-D3/6-31G(d)], see the Computational Details section.

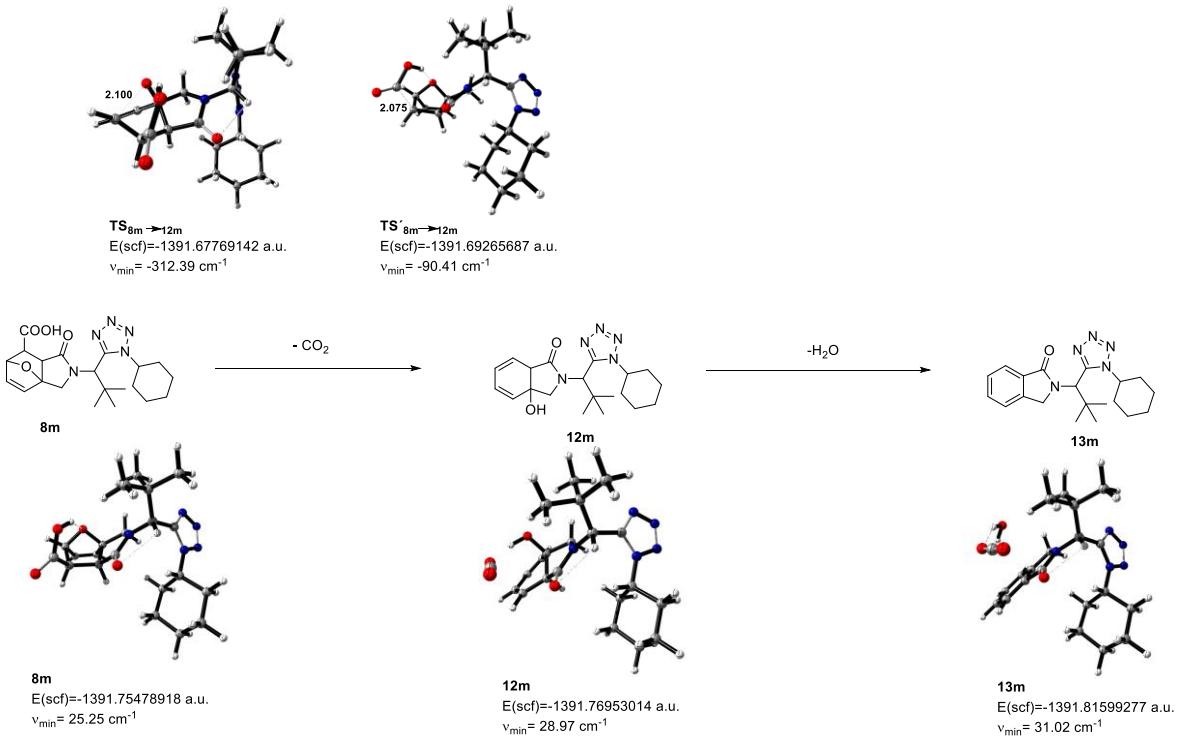
The first process studied was the reaction between Ugi-azide adduct **6m** and maleic anhydride **7** towards the oxa-bridged compound **8m**. In this context, we propose that the process can follow two major pathways: **a**) Diels-Alder / *N*-acylation or **b**) *N*-acylation / Diels-Alder. Besides, each Diels-Alder (DA) process can give *endo* or *exo* cycloadducts, resulting in four pathways.

Thus, the *endo* DA is the kinetically most favored route with an activation energy barrier of 18.6 Kcal/mol, which connects to the **9m<sup>(endo)</sup>** intermediate (**Scheme S2**). However, despite being an exergonic process of 4.2 Kcal/mol, it generates the thermodynamically less favored path among all of the possible routes. Besides, the second process of this pathway (*N*-acylation) proceeds with a very high activation energy barrier (53.6 Kcal/mol). It made us to discard this alternative.

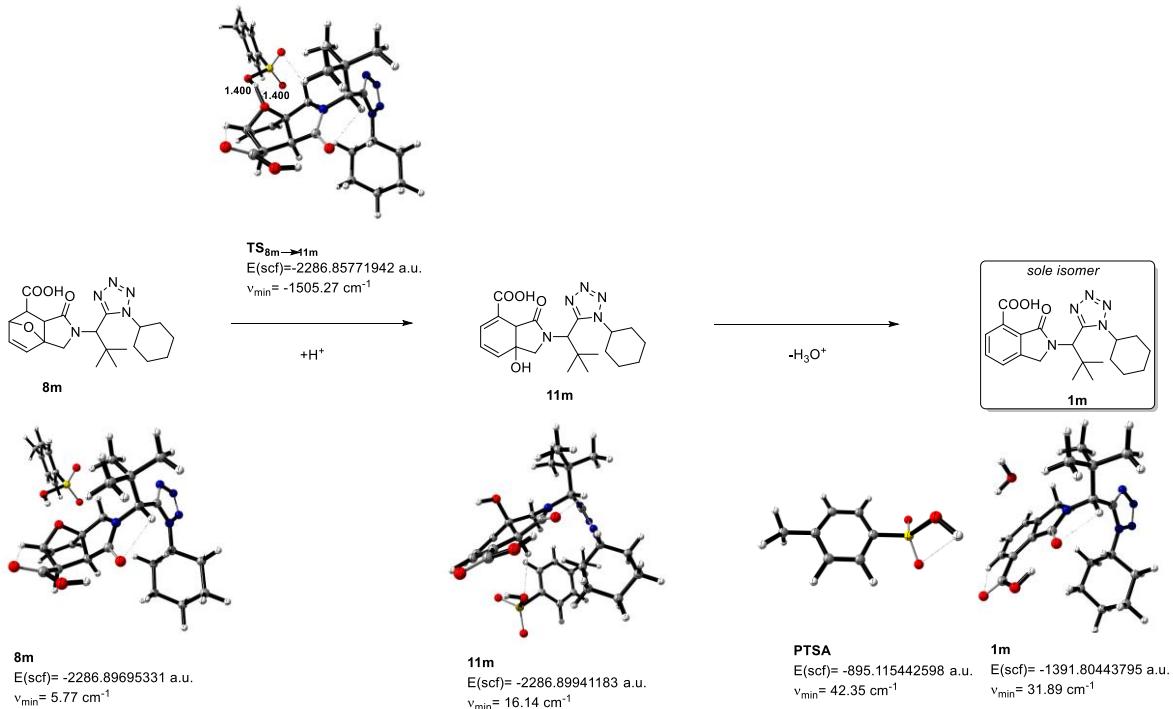
Moreover, the other route that leads to the intermediate **10m** with the proper conformation to subsequently follow the *endo* DA intramolecular step is the process favored thermodynamically by 10.5 Kcal/mol (**Scheme S3**). However, the activation energy for the intermediate **10m** is 28.0 Kcal/mol and is the kinetically less favored process among all of the proposed pathways. Besides, the second process of this alternative (*endo* DA intramolecular) requires a high energy activation of 35.6 Kcal/mol and the process is endergonic by 6.2 Kcal/mol (**10m** to **8m<sup>(endo)</sup>**). So this alternative was also discarded.

Finally, alternatives involving the *exo* Diels-Alder were analyzed. It was observed that intermediate **10m** is favored kinetically with an energy barrier of 21.5 Kcal/mol more than intermediate **9m<sup>(exo)</sup>**, which has an activation energy of 22.4 Kcal/mol (**Scheme S4**). Both processes are exergonic and favored thermodynamically by 6.0 Kcal/mol and 6.7 Kcal/mol respectively. Thus, at this stage we cannot conclude about the most favored pathway. However, analyzing the second stage we observed that the process from **10m** to **8m<sup>(exo)</sup>** is kinetic and thermodynamically favored since it requires only an activation energy of 7.2 Kcal/mol with respect to the process from **9m<sup>(exo)</sup>** to **8m** being the energy barrier much higher, *c.a.* 30.8 Kcal/mol (**Scheme S5**).

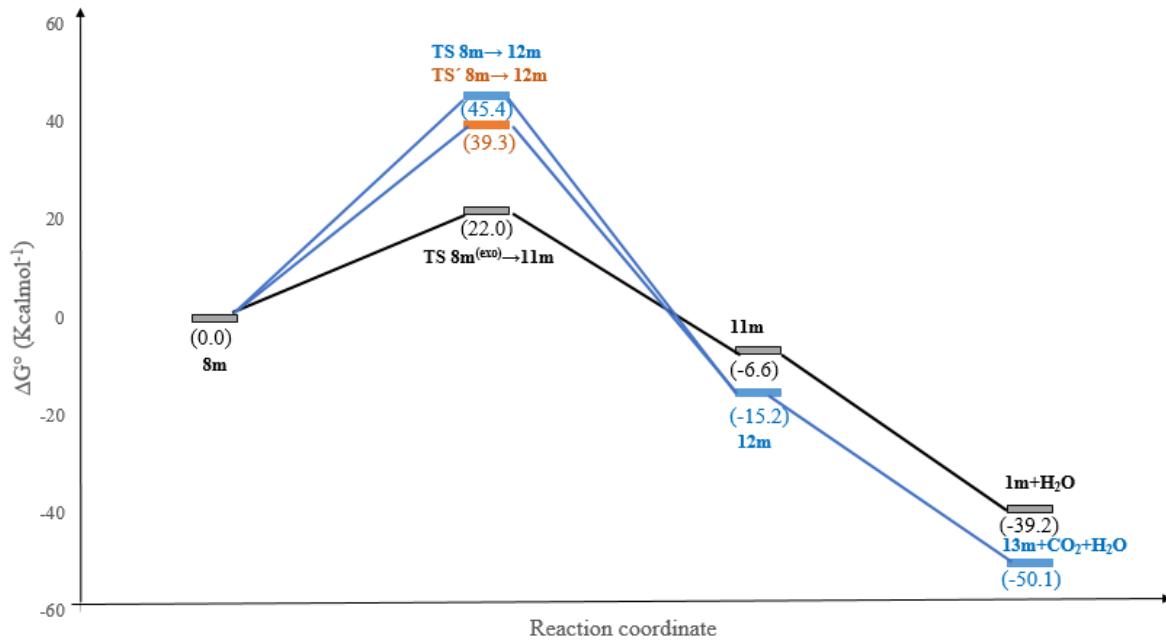
Additionally, product **8m** involving the *endo* DA is less stable than the product involving the *exo* DA by 8.6 Kcal/mol. Thus, the route *N*-acylation / *exo* Diels-Alder is the most thermodynamic and kinetically favored pathway (see **Figure S36**).



**Scheme S6.** Reaction path: **8m<sup>(exo)</sup>** → **12m** → **13m**.



**Scheme S7.** Reaction path: **8m<sup>(exo)</sup>** → **11m** → **1m**.



**Figure S37.** Energy profile for the whole route **8m** → **1m** or **13m**.

There are two possible reaction pathways from **8m**: *i*) decarboxylation / dehydration towards **13m**, and *ii*) dehydration towards **1m** (see **Scheme S1**).

There are two conformers of **8m**, one for each pathway (*i* and *ii*). The conformer **8m** involved in path *ii* is 0.54 Kcal/mol more stable than the rotamer involved in path *i*.

In the first process of path *i*, the decarboxylation process may occur through cleavage of the C3-O1 or the C1-C7 bond. Thus, two TS were located having 45.4 and 39.3 Kcal/mol (in relative Gibbs free energies), respectively. Both conditions led to intermediate **12m** (**Scheme S6**). This process is exergonic by 15.2 Kcal/mol. Finally, the dehydration process of **12m** allows the formation of the aromatized compound **13m**. Although the overall process is thermodynamically favored, it is noteworthy the high activation energy required (at least 39.3 Kcal/mol). For this reason, the product of this pathway (**13m**) was not detected experimentally.

For the pathway *ii*, it was proposed a dehydration step and further aromatization. This process is assisted by the *p*-toluene sulfonic acid protonating the *oxa*-compound **8m<sup>(exo)</sup>** involved in path *i*. This process occurs with an activation energy barrier of 22.0 Kcal/mol giving rise to the intermediate **11m** (**Scheme S7**). This process is exergonic by 6.6 Kcal/mol and the subsequent dehydration leads to **1m**, which was synthesized as the unique product. The overall process is exergonic by 39.2 Kcal/mol and we conclude that the process is favored by presenting the lower activation energy barriers (see the **Figure S37**).

Compound	HOMO	LUMO	Theoretical Values
<b>6j</b> 			gap <sub>HOMO-LUMO</sub> =3.15 eV $\lambda_{\text{abs}}=410.84 \text{ nm}$ $f=0.0853$ $E(\text{ev})= 3.0178$
<b>8j</b> 			gap <sub>HOMO-LUMO</sub> =3.16 eV $\lambda_{\text{abs}}=407.83 \text{ nm}$ $f=0.0842$ $E(\text{ev})= 3.0401$
<b>1j</b> 			gap <sub>HOMO-LUMO</sub> =3.07 eV $\lambda_{\text{abs}}=448.90 \text{ nm}, 403.20 \text{ nm}$ $f=0.0252, 0.0914$ $E(\text{ev})= 2.7619, 3.0750$

**Table S2.** TD-DFT calculations for the compounds **6j**, **8j** and **1j** where the wavelength for maximum absorbances, the vertical excitation energies and the oscillator strengths are shown.

The photophysical properties of the intermediates and one of the final products containing the anthracene moiety were examined using DFT calculations. Geometry optimizations, frequencies and absorption (TD-DFT) were calculated using the functional tHCTHhyb<sup>18</sup> in conjunction with the basis set 6-311g (d) using the Gaussian09 computational package.

The distribution of HOMO and LUMO in Ugi-Azide adduct **6j**, the oxa-bridged compound **8j** and the isoindolin-1-one **1j** are shown in **Table S2**. These molecules show fluorescent properties so we wanted to characterize better these systems. For **6j** and **8j**, the frontier orbitals are located exclusively on the anthracene ring. The theoretical estimation of the HOMO-LUMO gap for both structures is 3.15 and 3.16 eV, respectively, with an absorption band calculated at 410 and 407 nm, in the same order.

For the distribution of HOMO-LUMO in the structure containing the isoindolin-1-one core **1j**, it can be seen that this structure has very possibly an effective electron transfer because the HOMO is fully distributed on the anthracene ring, while the LUMO is located mostly on the isoindolinone core. The energy gap is 3.07 eV (which makes a slightly more favored electronic transition than the former molecules) and two absorption bands were located at 449 and 403nm. We can conclude that modifications in the isoindolin-1-one ring could affect the luminescent properties in this kind of *bis*-heterocycles as this can change the HOMO and LUMO distribution over the molecule.

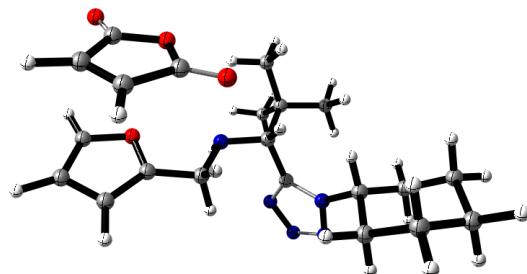
**Table S3.** Cartesian coordinates (xyz format) of all the structures involved in each reaction mechanism studied calculated at M06-2X/6-31G(d) level.

**6m+7 (connect to 9m<sup>(exo)</sup>)**

E(scf) = -1391.72597597 a.u.

v<sub>min</sub> = 15.76 cm<sup>-1</sup>

C	4.494699	-1.514388	-1.053724	N	-2.596028	1.136315	2.912652
C	3.259825	-2.012957	-1.069119	N	-3.373240	0.435245	2.168874
C	4.559360	-0.174753	1.587581	C	-3.361298	-0.523658	-0.064838
C	4.456977	-1.333961	2.291125	C	-3.456112	-1.985464	0.378458
C	2.434536	-0.701132	1.571652	C	-4.730386	0.040731	-0.447042
O	3.336512	0.219752	1.153702	H	-2.689703	-0.453159	-0.928393
C	0.991023	-0.462890	1.229230	C	-4.106861	-2.835139	-0.715593
H	0.643749	-1.246204	0.542196	H	-4.054751	-2.025146	1.296803
N	0.829518	0.814938	0.554356	H	-2.454457	-2.357605	0.623500
C	4.424983	-0.113635	-1.564800	C	-5.370165	-0.815940	-1.541989
C	2.354970	-0.972244	-1.637061	H	-5.362313	0.045526	0.449183
O	3.111489	0.139696	-1.919405	H	-4.619831	1.079932	-0.774928
H	5.424111	-1.962345	-0.732438	C	-5.478257	-2.278546	-1.105294
H	2.898311	-2.985893	-0.766706	H	-4.194840	-3.871326	-0.373391
O	5.288613	0.699429	-1.680820	H	-3.456172	-2.848270	-1.601063
O	1.183072	-1.039035	-1.868121	H	-6.357157	-0.414879	-1.793490
C	3.070477	-1.677157	2.283051	H	-4.760980	-0.754294	-2.454905
H	2.600477	-2.527943	2.755346	H	-5.918927	-2.882574	-1.905330
H	5.265750	-1.871930	2.763854	H	-6.154437	-2.347343	-0.242325
H	0.388573	-0.553356	2.148031	H	1.015570	1.562321	1.221885
C	-0.497603	1.002397	-0.012967	H	5.380589	0.475338	1.325968
H	-0.649914	0.178594	-0.723461				
C	-0.573947	2.325244	-0.828425				
C	0.387435	2.216580	-2.015582				
H	1.410940	2.045890	-1.674756				
H	0.111471	1.382588	-2.670150				
H	0.358751	3.141447	-2.602498				
C	-0.189496	3.530138	0.038700				
H	-0.788029	3.581172	0.953817				
H	0.870009	3.498799	0.314024				
H	-0.347459	4.454071	-0.527940				
C	-2.002842	2.516602	-1.349345				
H	-2.043975	3.394881	-2.001686				
H	-2.331234	1.652555	-1.942021				
H	-2.719055	2.674727	-0.534825				
C	-1.563279	0.921285	1.055264				
N	-2.747495	0.283541	0.990293				
N	-1.462296	1.454104	2.259134				

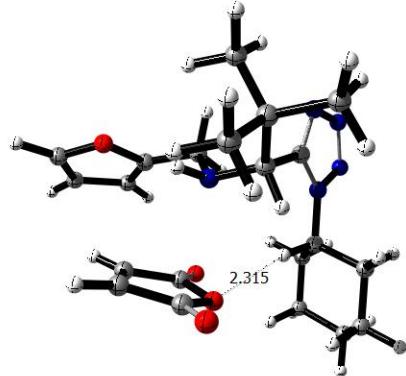


**6m+7 (connect to 10m)**

E(scf) = -1391.72818765 a.u.

 $\nu_{\min} = 26.53 \text{ cm}^{-1}$ 

C	2.154106	1.731935	2.220533	C	-2.679476	1.345055	-1.491786
C	2.114364	2.189430	0.971783	C	-3.599238	0.016541	0.460925
C	4.656560	0.948281	-1.122922	H	-1.550149	0.637932	0.187137
C	4.191349	1.877582	-1.996016	C	-3.153920	2.635842	-0.820183
C	2.583327	0.385650	-1.559444	H	-3.449954	0.960561	-2.170373
O	3.691979	0.033509	-0.848324	H	-1.774961	1.529603	-2.080737
C	1.390945	-0.490144	-1.385140	C	-4.065705	1.314886	1.122705
H	0.567367	-0.046159	-1.954653	H	-4.398407	-0.403800	-0.164084
N	1.032925	-0.525841	0.038183	H	-3.341914	-0.737546	1.214754
H	1.886047	-0.705290	0.564490	C	-4.370929	2.385872	0.072930
C	0.763073	1.376728	2.624480	H	-3.386445	3.382034	-1.587088
C	0.687017	2.180420	0.528579	H	-2.331698	3.041870	-0.217219
O	-0.080282	1.741810	1.594367	H	-4.945660	1.118376	1.743889
O	0.364668	0.859192	3.622763	H	-3.273792	1.677870	1.792306
C	2.832520	1.511811	-2.276528	H	-4.679935	3.316184	0.561529
H	2.124743	2.027503	-2.908633	H	-5.215851	2.054421	-0.546463
H	4.742627	2.715692	-2.396494	H	2.916372	2.514914	0.319546
H	1.584576	-1.487956	-1.807961	H	2.997871	1.578140	2.879454
C	0.015722	-1.514195	0.455788	H	5.606857	0.791916	-0.636393
H	-0.586288	-1.029249	1.241786	O	0.201588	2.520319	-0.507106
C	0.607503	-2.791055	1.116757				
C	1.291182	-2.365815	2.426162				
H	1.686114	-3.248994	2.938659				
H	2.142328	-1.691732	2.263875				
H	0.589268	-1.863548	3.101364				
C	1.630226	-3.489170	0.212696				
H	1.172001	-3.812146	-0.725308				
H	2.479352	-2.832383	-0.014990				
H	2.030190	-4.370300	0.726496				
C	-0.532095	-3.755458	1.467745				
H	-0.148214	-4.574531	2.084973				
H	-1.315093	-3.244558	2.042550				
H	-0.982769	-4.184882	0.570159				
C	-0.924010	-1.786468	-0.685679				
N	-1.922712	-0.958169	-1.046609				
N	-0.911179	-2.794367	-1.537039				
N	-1.921995	-2.573766	-2.398391				
N	-2.536437	-1.480253	-2.114200				
C	-2.384591	0.287970	-0.428349				

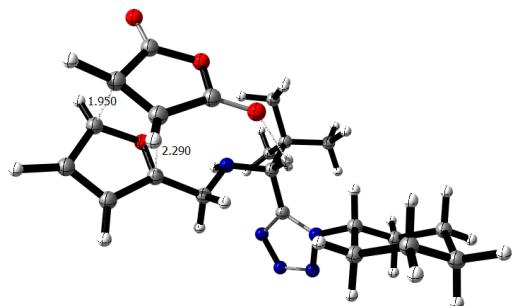


**TS<sub>[6m+7+7→9m<sup>(exo)</sup>]</sub>**

E(scf) = -1391.69296099 a.u.

ν<sub>min</sub> = -488.77 cm<sup>-1</sup>

C	4.284016	-1.378719	-0.497277	N	-3.340225	0.596700	2.142774
C	2.964423	-1.846846	-0.335409	C	-3.302536	-0.485331	-0.042731
C	4.608740	-0.238177	1.050696	C	-3.091376	-1.944648	0.366484
C	4.525361	-1.182645	2.122071	C	-4.779437	-0.163167	-0.269868
C	2.503959	-0.495313	1.454964	H	-2.750735	-0.290956	-0.968570
O	3.391352	0.395558	0.974583	C	-3.695874	-2.885673	-0.678053
C	1.049799	-0.123674	1.402412	H	-3.568444	-2.099930	1.342674
H	0.492710	-0.994605	1.038984	H	-2.018167	-2.135682	0.487386
N	0.848669	0.972961	0.470800	C	-5.368683	-1.110522	-1.317867
C	4.200477	-0.325648	-1.568066	H	-5.310414	-0.273295	0.682688
C	2.112042	-1.131875	-1.287309	H	-4.881834	0.882663	-0.580468
O	2.883208	-0.169974	-1.930779	C	-5.175935	-2.573232	-0.910771
H	5.170027	-2.002543	-0.493776	H	-3.566168	-3.924518	-0.358025
H	2.655163	-2.813391	0.034964	H	-3.147435	-2.774876	-1.623615
O	5.078675	0.329262	-2.044207	H	-6.431034	-0.887472	-1.458790
O	0.950232	-1.285380	-1.555296	H	-4.877456	-0.935260	-2.285253
C	3.188680	-1.378422	2.338936	H	-5.587178	-3.238236	-1.677316
H	2.711396	-2.110296	2.976665	H	-5.735509	-2.766245	0.014678
H	5.356276	-1.737974	2.534567	H	1.110890	1.852386	0.912687
H	0.684128	0.088990	2.420487	H	5.454122	0.385687	0.785529
C	-0.490287	1.068671	-0.085735				
H	-0.626442	0.173819	-0.708234				
C	-0.600863	2.303321	-1.023168				
C	0.516710	2.193370	-2.069422				
H	1.503339	2.294227	-1.619373				
H	0.487826	1.218444	-2.570995				
H	0.384788	2.979375	-2.822954				
C	-0.476357	3.626957	-0.226330				
H	-1.490670	4.106363	-0.081935				
H	-0.046449	3.468432	0.805758				
H	0.185787	4.350357	-0.782820				
C	-1.953221	2.266725	-1.746101				
H	-2.049203	3.143803	-2.393213				
H	-2.042544	1.376836	-2.380553				
H	-2.794910	2.283766	-1.037670				
C	-1.546069	1.061097	0.993710				
N	-2.726617	0.408610	0.964258				
N	-1.438497	1.642057	2.174750				
N	-2.563474	1.334946	2.851001				

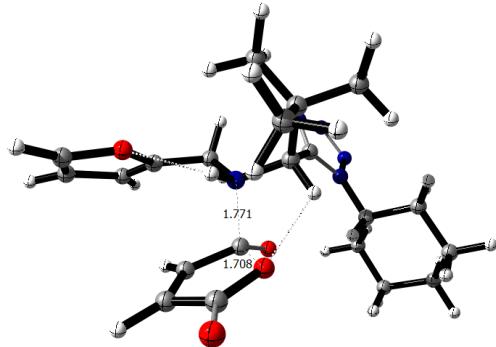


**TS<sub>[6m+7→10m]</sub>**

E(scf) = -1391.69521828 a.u.

ν<sub>min</sub> = -190.54 cm<sup>-1</sup>

C	2.378788	2.911380	0.142369	C	-3.375898	0.760959	-1.662132
C	1.978570	2.148248	-0.867556	C	-4.067730	-0.271259	0.544856
C	5.191882	-0.084596	-0.409439	H	-2.217829	0.784587	0.134413
C	5.303492	-0.017897	-1.758325	C	-4.190494	2.011113	-1.320115
C	3.214593	-0.580938	-1.207536	H	-3.994368	0.048115	-2.220696
O	3.926878	-0.435239	-0.058224	H	-2.504170	1.011779	-2.271581
C	1.786344	-0.967525	-1.042061	C	-4.889184	0.978138	0.872741
H	1.218508	-0.748936	-1.951770	H	-4.692739	-1.012329	0.030165
N	1.177877	-0.179530	0.067430	H	-3.690370	-0.742196	1.460424
H	1.887744	-0.021721	0.788026	C	-5.368834	1.672733	-0.403957
C	1.454137	2.793387	1.320069	H	-4.545683	2.480603	-2.243174
C	0.708396	1.408724	-0.559983	H	-3.536578	2.741229	-0.823945
O	0.436964	1.995118	1.021334	H	-5.739051	0.705433	1.506726
O	1.628913	3.325749	2.390603	H	-4.269096	1.674983	1.453209
C	4.007397	-0.339623	-2.282365	H	-5.929133	2.579315	-0.152276
H	3.706444	-0.380443	-3.319414	H	-6.060210	1.006325	-0.937934
H	6.192187	0.233505	-2.317463	H	2.428079	2.056621	-1.848826
H	1.674028	-2.035000	-0.838202	H	3.242922	3.563080	0.171233
C	-0.025409	-0.789279	0.724808	H	5.878062	0.077589	0.406663
H	-0.585924	0.069309	1.108485	O	-0.262838	1.29267	-1.266953
C	0.360166	-1.641342	1.971921				
C	0.929702	-0.688492	3.055484				
H	1.776873	-1.181834	3.617420				
H	1.295721	0.293981	2.634858				
H	0.118551	-0.420710	3.800599				
C	1.389599	-2.737508	1.646811				
H	1.026441	-3.407999	0.863604				
H	2.355039	-2.311990	1.347074				
H	1.566248	-3.327667	2.551655				
C	-0.917920	-2.300785	2.507604				
H	-0.701330	-2.786778	3.463622				
H	-1.697995	-1.549795	2.684318				
H	-1.301580	-3.056026	1.820153				
C	-0.889870	-1.506797	-0.261975				
N	-2.107412	-1.105158	-0.677481				
N	-0.641484	-2.678424	-0.819691				
N	-1.715799	-2.975423	-1.574121				
N	-2.600373	-2.045052	-1.488687				
C	-2.899357	0.093972	-0.371816				

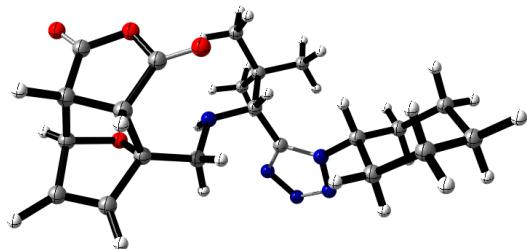


**9m<sup>(exo)</sup>**

E(scf) = -1391.74426175 a.u.

ν<sub>min</sub> = 16.59 cm<sup>-1</sup>

C	-4.380797	-0.880212	0.779668	N	3.267011	-0.468074	-2.216335
C	-2.903454	-1.260437	0.914223	C	3.385928	-0.420971	0.213331
C	-4.578108	-0.919672	-0.770703	C	3.428930	-1.932592	0.448227
C	-4.388032	-2.360227	-1.221999	C	4.786008	0.193331	0.233130
C	-2.474441	-1.287225	-0.609851	H	2.781550	0.045828	0.999258
O	-3.354776	-0.315501	-1.168914	C	4.133372	-2.246541	1.769829
C	-1.030840	-0.927291	-0.888404	H	3.966147	-2.395043	-0.389204
H	-0.393350	-1.482359	-0.187764	H	2.407814	-2.331888	0.442874
N	-0.864231	0.499873	-0.649278	C	5.483270	-0.126902	1.557344
C	-4.409066	0.568310	1.243145	H	5.356235	-0.219712	-0.607495
C	-2.289256	-0.122765	1.697736	H	4.712978	1.275492	0.078716
O	-3.184012	0.923737	1.765364	C	5.536401	-1.636458	1.806016
H	-5.096527	-1.480600	1.343569	H	4.181181	-3.330624	1.914332
H	-2.679018	-2.204205	1.411353	H	3.540324	-1.842031	2.601870
O	-5.316177	1.337613	1.182971	H	6.492014	0.298143	1.553784
O	-1.236312	-0.095275	2.260857	H	4.939026	0.357457	2.380254
C	-3.077477	-2.586043	-1.133871	H	6.016200	-1.845359	2.767835
H	-2.532883	-3.509301	-1.291491	H	6.154702	-2.107698	1.029981
H	-5.181453	-3.051625	-1.475638	H	-1.180498	1.004933	-1.473807
H	-0.750518	-1.229799	-1.906785	H	-5.436867	-0.358274	-1.135514
C	0.484976	0.909542	-0.293889				
H	0.702141	0.438902	0.675949				
C	0.563557	2.448499	-0.079191				
C	-0.369571	2.829133	1.074685				
H	-1.407906	2.583918	0.839483				
H	-0.103433	2.295583	1.993194				
H	-0.301279	3.905930	1.265213				
C	0.152506	3.210088	-1.346054				
H	0.732408	2.897079	-2.219775				
H	-0.911512	3.076924	-1.569061				
H	0.312869	4.282515	-1.192215				
C	2.002109	2.832685	0.287324				
H	2.052634	3.903386	0.509827				
H	2.344436	2.296328	1.181752				
H	2.701670	2.631454	-0.532324				
C	1.495856	0.413480	-1.300920				
N	2.705135	-0.123425	-1.046861				
N	1.318346	0.397698	-2.609046				
N	2.430871	-0.148405	-3.136916				

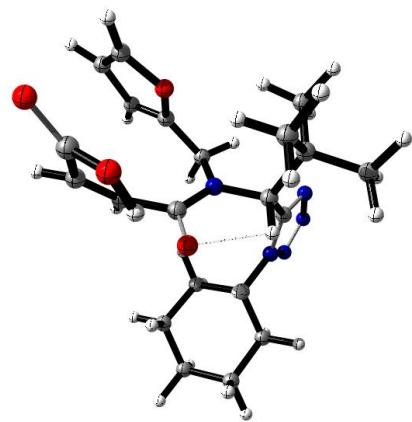


**10m**

E(scf) = -1391.74026288 a.u.

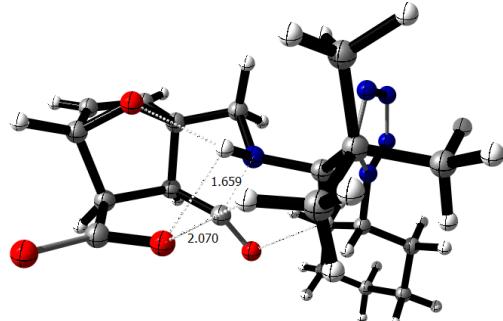
 $\nu_{\min} = 24.22 \text{ cm}^{-1}$ 

C	2.560347	-2.354607	-0.033098	N	-3.567327	1.373031	1.263681
C	1.394266	-1.822357	0.342765	C	-2.866881	-0.600448	-0.007330
C	4.250159	0.276058	1.103913	C	-2.455838	-1.562692	1.109128
C	4.196780	-0.156093	2.388992	C	-4.295046	-0.872840	-0.477836
C	2.159674	0.454476	1.714301	H	-2.181587	-0.736002	-0.853400
O	3.019250	0.669646	0.687817	C	-2.554542	-3.005313	0.608386
C	0.709963	0.713326	1.456987	H	-3.119915	-1.403925	1.968718
H	0.122722	0.157791	2.201485	H	-1.435289	-1.330237	1.437772
N	0.303025	0.352414	0.092999	C	-4.406154	-2.319830	-0.968350
H	1.827598	-1.614506	-2.266659	H	-4.981490	-0.699189	0.358951
C	3.405519	-1.980313	-1.221319	H	-4.562280	-0.166824	-1.271123
C	0.605288	-0.842088	-0.473068	C	-3.970271	-3.312464	0.112870
O	2.804925	-1.564932	-2.336419	H	-2.267480	-3.698111	1.406131
O	4.606427	-2.050495	-1.140698	H	-1.837031	-3.145287	-0.212921
O	0.232565	-1.143650	-1.613020	H	-5.435036	-2.523276	-1.281299
C	2.826678	-0.040685	2.789389	H	-3.772265	-2.450131	-1.856112
H	2.392408	-0.314014	3.740738	H	-4.022428	-4.336115	-0.271630
H	5.024862	-0.524998	2.975258	H	-4.667093	-3.252875	0.959878
H	0.456440	1.768098	1.589833	H	0.965214	-2.108202	1.301835
C	-0.519900	1.304104	-0.677022	H	3.066006	-3.046650	0.633035
H	-0.891855	0.721872	-1.524221	H	5.037358	0.34523	0.369603
C	0.267013	2.480700	-1.312173				
C	1.304493	1.870376	-2.264265				
H	0.828077	1.245866	-3.027971				
H	1.852416	2.672156	-2.769659				
H	2.032311	1.254773	-1.725531				
C	0.984860	3.385466	-0.302544				
H	0.293897	3.794447	0.440445				
H	1.804276	2.861177	0.199650				
H	1.432337	4.225946	-0.844224				
C	-0.733241	3.319543	-2.119483				
H	-0.190652	4.070174	-2.702928				
H	-1.299033	2.696973	-2.823279				
H	-1.438727	3.839495	-1.465806				
C	-1.707806	1.662091	0.170230				
N	-2.705141	0.789676	0.423211				
N	-1.955881	2.765814	0.844804				
N	-3.113429	2.552395	1.502328				



**TS<sub>[9m]<sup>(exo)</sup> → 8m]</sub>**  
E(scf) = -1391.69091807 a.u.  
v<sub>min</sub> = -157.49 cm<sup>-1</sup>

C	3.419019	-1.646649	-0.488515	N	-3.107607	0.687125	1.981183
C	2.052225	-1.569416	0.199154	C	-2.943829	-0.594144	-0.082641
C	4.303752	-0.900230	0.565533	C	-2.762943	-1.969335	0.561272
C	4.272198	-1.628580	1.903405	C	-4.395851	-0.335673	-0.483191
C	2.364857	-0.569728	1.375799	H	-2.302505	-0.543519	-0.967460
O	3.429939	0.202613	0.835944	C	-3.245341	-3.059155	-0.398271
C	1.166875	0.337276	1.514813	H	-3.338872	-1.995629	1.494925
H	0.306413	-0.175970	1.959804	H	-1.705174	-2.113874	0.809421
N	0.861761	0.617848	0.074976	C	-4.871939	-1.433507	-1.438856
C	3.436032	-0.749549	-1.758074	H	-5.013463	-0.327142	0.422694
C	0.979514	-0.886734	-0.614312	H	-4.479625	0.653875	-0.946457
O	2.337724	-0.108079	-1.968962	C	-4.698570	-2.821424	-0.816527
H	3.765121	-2.655672	-0.714656	H	-3.137022	-4.040248	0.074750
H	1.655609	-2.524564	0.548479	H	-2.599330	-3.060489	-1.286426
O	4.479961	-0.673397	-2.382882	H	-5.918886	-1.258484	-1.705653
O	-0.004071	-1.310091	-1.139198	H	-4.292686	-1.380206	-2.370779
C	3.071334	-1.389798	2.437377	H	-5.020708	-3.594135	-1.522063
H	2.627307	-1.798297	3.336045	H	-5.347255	-2.903144	0.066305
H	5.054520	-2.272951	2.283937	H	1.682114	1.089994	-0.338708
H	1.369124	1.256574	2.062209	H	5.260139	-0.562949	0.171230
C	-0.391550	1.330341	-0.325336				
H	-0.771010	0.741716	-1.166958				
C	-0.119761	2.763532	-0.854690				
C	0.659303	2.649524	-2.176394				
H	1.622864	2.145032	-2.075836				
H	0.085172	2.093678	-2.923474				
H	0.844801	3.657229	-2.565534				
C	0.663617	3.630234	0.162993				
H	0.169677	4.641110	0.268940				
H	0.664618	3.166494	1.196351				
H	1.727931	3.788231	-0.183748				
C	-1.489064	3.391426	-1.154936				
H	-1.341719	4.348018	-1.669171				
H	-2.089032	2.751012	-1.812361				
H	-2.056648	3.585866	-0.243473				
C	-1.396464	1.269090	0.780529				
N	-2.466176	0.452910	0.830588				
N	-1.380800	1.992578	1.883810				
N	-2.451521	1.605977	2.598537				

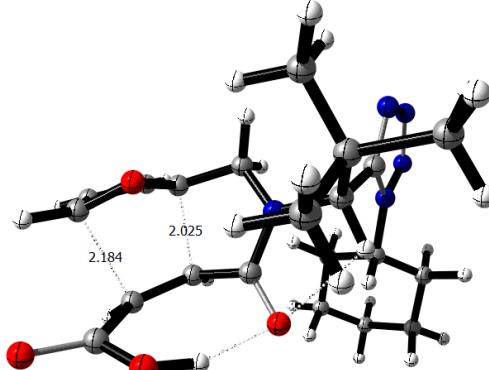


**TS<sub>[10m → 8m<sup>(exo)</sup>]</sub>**

E(scf) = -1391.70760017 a.u.

ν<sub>min</sub> = -550.35 cm<sup>-1</sup>

C	3.021046	-1.701716	-0.206159	C	-2.750754	-0.800187	-0.180614
C	1.690260	-1.424704	0.157085	C	-2.221014	-1.886792	0.758104
C	3.986251	-0.382665	1.242151	C	-4.147900	-1.142158	-0.697856
C	3.735077	-1.136247	2.411978	H	-2.064245	-0.709513	-1.031856
C	1.905732	-0.106230	1.679234	C	-2.188016	-3.233098	0.031225
O	2.970021	0.503591	1.073784	H	-2.877200	-1.936662	1.636698
C	0.597217	0.596407	1.527307	H	-1.219464	-1.611717	1.112606
H	-0.166995	0.093331	2.136062	C	-4.119751	-2.494106	-1.416425
N	0.270695	0.530017	0.103829	H	-4.836965	-1.177306	0.154034
H	2.166027	-0.743203	-2.332685	H	-4.495989	-0.347818	-1.366471
C	3.797187	-1.147245	-1.370587	C	-3.574746	-3.597194	-0.505556
C	0.766465	-0.510661	-0.613406	H	-1.820975	-4.011700	0.707936
O	3.126861	-0.554311	-2.366262	H	-1.474930	-3.169933	-0.803035
O	5.001662	-1.228217	-1.409158	H	-5.127177	-2.746323	-1.761903
O	0.458156	-0.709077	-1.791172	H	-3.487021	-2.417720	-2.311107
C	2.406542	-0.944904	2.708110	H	-3.533186	-4.548337	-1.045942
H	1.805344	-1.452046	3.450497	H	-4.261313	-3.738549	0.340104
H	4.430948	-1.822191	2.873838	H	1.136589	-2.234387	0.631702
H	0.644684	1.637874	1.850691	H	3.437346	-2.648899	0.118373
C	-0.669532	1.471703	-0.510653	H	4.926082	-0.135132	0.768341
H	-0.972259	0.989241	-1.445903				
C	-0.033999	2.822369	-0.932093				
C	1.038101	2.510062	-1.985319				
H	0.614010	1.982873	-2.846974				
H	1.485251	3.444296	-2.340151				
H	1.843067	1.891954	-1.572598				
C	0.619228	3.590162	0.222925				
H	-0.080255	3.759912	1.046630				
H	1.510474	3.069014	0.589815				
H	0.951848	4.566364	-0.145910				
C	-1.136702	3.681507	-1.563573				
H	-0.691085	4.574837	-2.012696				
H	-1.659432	3.136073	-2.358757				
H	-1.869897	4.002175	-0.818620				
C	-1.876920	1.531240	0.380056				
N	-2.744661	0.504121	0.486945				
N	-2.236725	2.457813	1.243344				
N	-3.334942	1.983496	1.866749				
N	-3.644300	0.815175	1.428296				

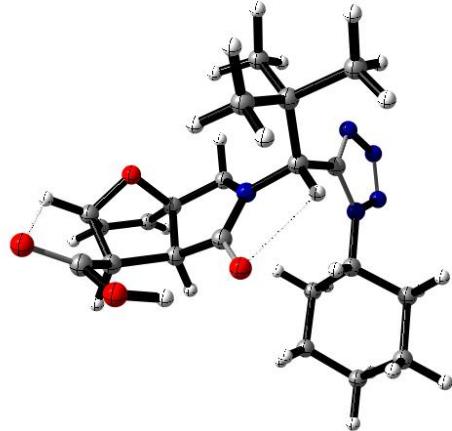


**8m<sup>(exo)</sup>** (*involved in path ii*)

E(scf) = -1391.75564962 a.u.

v<sub>min</sub> = 21.63 cm<sup>-1</sup>

C	3.225914	-1.366316	-0.005333	N	-3.717603	0.656727	1.361450
C	1.734082	-1.144067	0.369936	C	-2.634588	-0.923962	-0.162731
C	3.905281	-0.447178	1.069010	C	-2.084303	-1.943927	0.836767
C	3.701812	-1.078168	2.439526	C	-3.964670	-1.388719	-0.755265
C	1.862835	-0.128360	1.555015	H	-1.907278	-0.804348	-0.975021
O	2.974904	0.634554	1.101380	C	-1.884430	-3.292801	0.142243
C	0.599308	0.701073	1.526509	H	-2.796127	-2.037837	1.667025
H	-0.191019	0.269238	2.155414	H	-1.139835	-1.577231	1.258232
N	0.232103	0.634864	0.109620	C	-3.772850	-2.744264	-1.442876
C	3.774501	-1.010781	-1.398867	H	-4.702075	-1.469688	0.051907
C	0.787637	-0.403444	-0.558210	H	-4.334689	-0.638793	-1.462183
O	3.007888	-1.221370	-2.464554	C	-3.195019	-3.783974	-0.478431
H	3.495619	-2.417435	0.142027	H	-1.497823	-4.027056	0.856546
H	1.240650	-2.080958	0.651856	H	-1.126315	-3.177166	-0.645882
O	4.918817	-0.654685	-1.515453	H	-4.728725	-3.089806	-1.848562
O	0.500430	-0.728315	-1.711232	H	-3.090411	-2.623416	-2.295193
C	2.425014	-0.860475	2.755807	H	-3.034280	-4.733813	-0.998411
H	1.858051	-1.212269	3.608717	H	-3.921491	-3.976223	0.322632
H	4.443082	-1.653149	2.980007	H	4.899787	-0.113330	0.785445
H	0.780201	1.725796	1.849820	H	2.051647	-1.305885	-2.248144
C	-0.755372	1.508245	-0.521722				
H	-1.005965	1.002172	-1.461756				
C	-0.203329	2.897549	-0.933932				
C	0.938959	2.651948	-1.928760				
H	1.767411	2.112165	-1.456397				
H	0.601932	2.073367	-2.795902				
H	1.327644	3.610816	-2.286065				
C	0.333330	3.727028	0.239714				
H	-0.400965	3.818915	1.044997				
H	1.265478	3.305588	0.630995				
H	0.569110	4.734470	-0.120133				
C	-1.337165	3.662122	-1.629048				
H	-0.942272	4.587719	-2.059536				
H	-1.770942	3.073579	-2.446625				
H	-2.131419	3.923481	-0.924804				
C	-1.984959	1.490452	0.342406				
N	-2.762436	0.394112	0.462605				
N	-2.456014	2.411991	1.155809				
N	-3.528512	1.863411	1.762994				

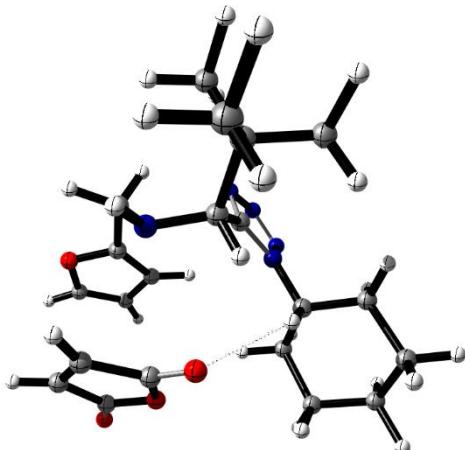


**6m+7 (connect to 9m<sup>(endo)</sup>)**

E(scf) = -1391.72401989 a.u.

v<sub>min</sub> = 20.74 cm<sup>-1</sup>

C	-2.616205	-0.170090	-1.818791	N	1.450811	-0.733623	2.854145
C	-1.927690	-1.683632	0.783621	C	1.789757	1.548936	0.230049
C	-3.977183	-1.083181	1.282869	C	0.798589	2.640829	0.632402
C	-3.821917	0.218462	-1.406550	C	3.233237	2.039013	0.348903
H	-2.303672	-1.067504	-2.330924	H	1.583178	1.254615	-0.801765
H	-4.779321	-0.274995	-1.498459	C	0.988657	3.859243	-0.271391
C	-1.831423	-0.521465	1.495526	H	0.981833	2.908530	1.680438
C	-3.167784	-0.130190	1.816839	H	-0.223147	2.257714	0.556956
H	-5.045359	-1.237374	1.283439	C	3.432453	3.268146	-0.542954
C	-3.677614	1.539900	-0.733086	H	3.430596	2.293206	1.397761
C	-1.648852	0.905693	-1.471077	H	3.925668	1.236010	0.071222
O	-4.497740	2.243273	-0.232037	C	2.429252	4.374103	-0.202485
O	-2.335802	1.890862	-0.792328	H	0.285227	4.646617	0.017375
O	-3.237783	-2.032286	0.660448	H	0.741335	3.573121	-1.302586
H	-0.927401	-0.011107	1.795828	H	4.458699	3.636126	-0.441900
H	-3.480665	0.745775	2.366434	H	3.302952	2.973946	-1.593923
C	-0.948241	-2.624908	0.142406	H	2.563350	5.223940	-0.880265
H	-0.314992	-3.072071	0.915043	H	2.631386	4.740805	0.813236
H	-1.539365	-3.428688	-0.307348	O	-0.488692	1.016916	-1.739045
N	-0.171362	-1.978446	-0.924793	H	-0.141131	-2.580018	-1.740857
C	1.194131	-1.510473	-0.654057				
H	1.367262	-0.682799	-1.354878				
C	2.328625	-2.549569	-0.938238				
C	2.343348	-2.849148	-2.443681				
H	3.174373	-3.521330	-2.681055				
H	1.427794	-3.350712	-2.778836				
H	2.468622	-1.933804	-3.033587				
C	2.130758	-3.858269	-0.168373				
H	2.106951	-3.689983	0.911270				
H	1.198551	-4.353600	-0.464278				
H	2.953110	-4.545587	-0.396067				
C	3.674039	-1.918750	-0.560327				
H	4.498073	-2.571380	-0.866749				
H	3.810052	-0.952083	-1.062931				
H	3.754926	-1.760730	0.520210				
C	1.317719	-0.937422	0.729712				
N	1.242698	-1.615225	1.863570				
N	1.580144	0.347730	1.045423				
N	1.656179	0.443829	2.379224				

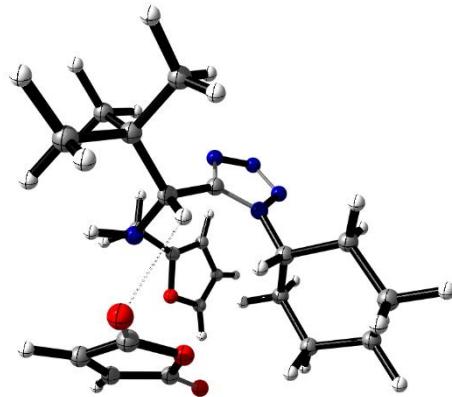


**6m+7 (connect to 10m)**

E(scf) = -1391.73195912 a.u.

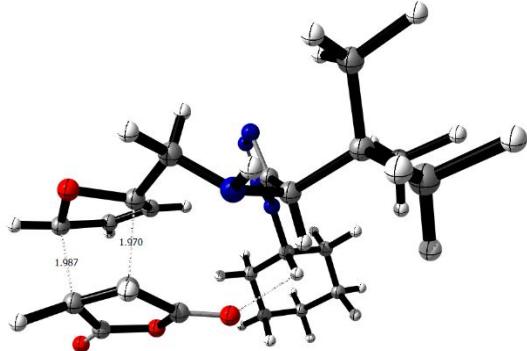
v<sub>min</sub> = 27.84 cm<sup>-1</sup>

C	1.421708	-1.439154	1.552781	H	1.327902	0.225898	-1.371326
H	2.208990	-0.881346	2.073071	C	-0.181672	-2.071869	-1.952721
N	1.425664	-1.236353	0.093430	O	0.548890	-1.543651	-2.735982
C	1.849625	0.085071	-0.414920	C	-0.122268	-3.436467	-1.354269
C	3.366231	0.194768	-0.766987	C	-1.209795	-3.606203	-0.608941
C	4.274774	-0.216243	0.396456	C	-2.021020	-2.358321	-0.693574
H	4.104794	0.410386	1.275519	O	-1.338127	-1.468949	-1.501182
H	4.118536	-1.266082	0.673994	O	-3.083509	-2.101997	-0.216108
H	5.322883	-0.114714	0.093508	H	0.698645	-4.113144	-1.551763
C	3.639020	-0.720289	-1.970638	H	-1.523665	-4.452692	-0.014225
H	3.437388	-1.776990	-1.755834	H	1.606760	-2.507249	1.718789
H	3.026612	-0.439113	-2.833312	C	0.116721	-1.084427	2.184032
H	4.694158	-0.649747	-2.255004	C	-0.246938	-0.182156	3.133478
C	3.676728	1.637188	-1.186257	O	-0.962679	-1.841421	1.828958
H	3.626462	2.320752	-0.334911	C	-1.643228	-0.394351	3.382007
H	4.684588	1.694304	-1.610677	H	0.400977	0.552937	3.589906
H	2.972284	1.983407	-1.953390	C	-2.021366	-1.406016	2.563436
C	1.376446	1.170927	0.505931	H	-2.275709	0.147066	4.069654
N	1.996426	1.619765	1.583114	H	-2.961335	-1.895777	2.361226
N	1.203932	2.569529	2.108202	H	2.049513	-1.925054	-0.320222
N	0.137977	2.715776	1.403276				
N	0.223877	1.854758	0.383136				
C	-0.884289	1.744085	-0.572733				
C	-2.106915	1.147372	0.124206				
C	-1.178747	3.112046	-1.190820				
H	-0.549091	1.051213	-1.353772				
C	-3.299596	1.084105	-0.830855				
H	-2.346694	1.771497	0.995049				
H	-1.853226	0.150510	0.497217				
C	-2.371943	3.020004	-2.144454				
H	-1.401122	3.816440	-0.380437				
H	-0.285650	3.480834	-1.708290				
C	-3.603862	2.457567	-1.431344				
H	-4.168189	0.683644	-0.298720				
H	-3.077164	0.375468	-1.638279				
H	-2.583209	4.009794	-2.562510				
H	-2.114117	2.366695	-2.989740				
H	-4.445374	2.389378	-2.129215				
H	-3.905341	3.149675	-0.632786				



**TS<sub>[6m+7→9m<sup>(endo)</sup>]</sub>**  
E(scf) = -1391.69941046 a.u.  
v<sub>min</sub> = -529.06 cm<sup>-1</sup>

C	-2.463286	-0.688592	-1.208350	N	1.401201	-0.612768	2.879423
C	-1.898568	-1.561000	0.465225	C	1.651693	1.630626	0.211042
C	-3.910660	-0.980794	0.984969	C	0.551681	2.636509	0.546930
C	-3.809502	-0.291817	-0.876402	C	3.035285	2.261322	0.368737
H	-2.220630	-1.486286	-1.902525	H	1.512786	1.295812	-0.819968
H	-4.687617	-0.755362	-1.311191	C	0.655137	3.837897	-0.394098
C	-1.784079	-0.423499	1.377951	H	0.677595	2.954254	1.589424
C	-3.047569	-0.059143	1.695765	H	-0.431883	2.164461	0.453238
H	-4.949770	-1.184041	1.220939	C	3.155300	3.476323	-0.555470
C	-3.799752	1.188556	-0.786898	H	3.163733	2.564612	1.418326
C	-1.688368	0.569302	-1.353754	H	3.815754	1.522577	0.148666
O	-4.685590	1.959652	-0.565648	C	2.036375	4.490733	-0.295876
O	-2.491341	1.625294	-0.961077	H	-0.127762	4.562743	-0.156377
O	-3.157411	-2.088447	0.692065	H	0.473839	3.491718	-1.419831
H	-0.868324	0.090226	1.648042	H	4.134261	3.945134	-0.429729
H	-3.373273	0.810304	2.250198	H	3.096592	3.135700	-1.601652
C	-0.853923	-2.614523	0.155673	H	2.118084	5.326059	-1.000560
H	-0.371880	-2.923134	1.090462	H	2.164768	4.912595	0.709649
H	-1.418128	-3.466660	-0.235484	O	-0.558301	0.755899	-1.710084
N	0.077781	-2.212216	-0.893322	H	0.294365	-3.022604	-1.468122
C	1.323150	-1.481139	-0.617563				
H	1.357968	-0.645216	-1.330318				
C	2.611489	-2.329924	-0.885263				
C	2.655856	-2.680366	-2.379814				
H	3.587298	-3.214459	-2.607394				
H	1.836175	-3.336864	-2.694919				
H	2.621276	-1.779678	-3.002888				
C	2.630731	-3.610109	-0.048926				
H	2.617254	-3.388365	1.020370				
H	1.767047	-4.248767	-0.273712				
H	3.534572	-4.186636	-0.274031				
C	3.839066	-1.471526	-0.563834				
H	4.755040	-1.996447	-0.859697				
H	3.806453	-0.518359	-1.109747				
H	3.913016	-1.254749	0.508547				
C	1.358815	-0.877308	0.757635				
N	1.291290	-1.531030	1.902663				
N	1.523818	0.431913	1.047040				
N	1.541526	0.564541	2.380220				

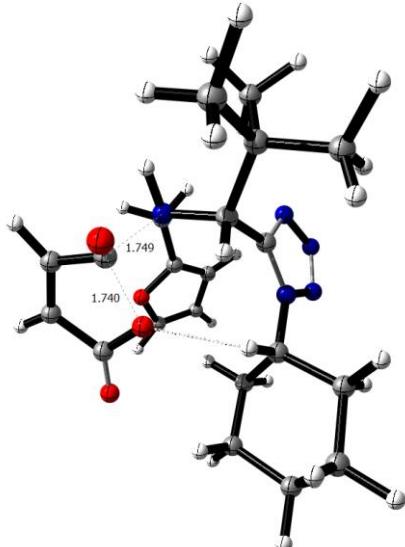


**TS<sub>[6m+7→10m]</sub>**

E(scf) = -1391.68888851 a.u.

ν<sub>min</sub> = -161.72 cm<sup>-1</sup>

C	-1.433381	1.627823	1.229673	H	-1.185769	-0.595277	-1.264677
H	-2.103803	1.146622	1.946875	C	-1.078002	1.772676	-1.577713
N	-1.749521	1.053504	-0.131776	O	-1.601874	1.271094	-2.538254
C	-1.721751	-0.448554	-0.322822	C	-0.849847	3.240956	-1.378330
C	-3.149438	-1.053488	-0.516523	C	0.438436	3.537458	-1.276434
C	-4.104745	-0.726028	0.664314	C	1.294413	2.300614	-1.221996
H	-4.689905	-1.647366	0.940437	O	0.541315	1.218195	-1.264722
H	-3.554144	-0.414865	1.588065	O	2.502119	2.317030	-1.121183
H	-4.844625	0.072625	0.368686	H	-1.683096	3.930044	-1.467483
C	-3.772943	-0.531804	-1.821254	H	0.883387	4.523387	-1.221866
H	-3.910732	0.557806	-1.825861	H	-1.714646	2.683179	1.154233
H	-3.162785	-0.779503	-2.691342	C	-0.050616	1.536357	1.778278
H	-4.764863	-0.983970	-1.934349	C	0.470919	0.837919	2.826843
C	-2.978260	-2.573342	-0.668044	O	0.860331	2.445381	1.342604
H	-2.659978	-3.045512	0.267542	C	1.802558	1.323538	3.015123
H	-3.936292	-3.015622	-0.960912	H	-0.028128	0.068729	3.397185
H	-2.244098	-2.809071	-1.451568	C	1.983025	2.288991	2.078790
C	-0.981106	-1.149683	0.772576	H	2.525021	0.982713	3.741201
N	-1.474041	-1.451232	1.963575	H	2.815794	2.911774	1.790912
N	-0.527447	-2.162478	2.591192	H	-2.727768	1.317098	-0.288239
N	0.511774	-2.305404	1.843174				
N	0.248826	-1.685997	0.689106				
C	1.273234	-1.632512	-0.364798				
C	2.470343	-0.807521	0.105374				
C	1.678515	-3.045529	-0.784290				
H	0.811812	-1.109033	-1.206821				
C	3.514333	-0.740961	-1.008985				
H	2.888671	-1.278745	1.005170				
H	2.139063	0.200265	0.369112				
C	2.732876	-2.970634	-1.892998				
H	2.086096	-3.567968	0.089864				
H	0.795062	-3.603246	-1.117507				
C	3.942482	-2.141225	-1.452360				
H	4.374357	-0.156742	-0.667805				
H	3.085826	-0.187401	-1.853953				
H	3.038562	-3.982759	-2.177933				
H	2.286112	-2.509686	-2.784747				
H	4.670685	-2.078059	-2.268118				
H	4.441649	-2.652071	-0.617119				

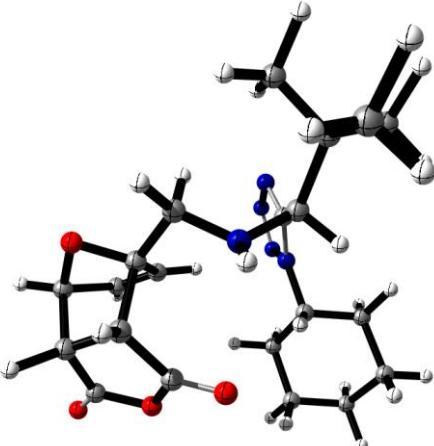


**9m<sup>(endo)</sup>**

E(scf) = -1391.73836760 a.u.

ν<sub>min</sub> = 28.80 cm<sup>-1</sup>

C	2.235208	1.155623	-1.131488	N	-1.777243	0.104766	2.959401
C	1.376959	1.807901	0.034908	C	-1.024712	-1.952448	0.214216
C	3.365212	2.079878	0.780567	C	0.222913	-2.675615	0.724619
C	3.649382	1.299482	-0.561226	C	-2.193093	-2.920276	0.013247
H	2.057214	1.703887	-2.059350	H	-0.770207	-1.459809	-0.731381
H	4.348702	1.843125	-1.198507	C	0.611444	-3.791979	-0.248173
C	1.488728	0.904593	1.256801	H	0.013364	-3.090024	1.717672
C	2.718415	1.090365	1.735495	H	1.047122	-1.961379	0.834931
H	4.188017	2.692300	1.142441	C	-1.797292	-4.037872	-0.953437
C	4.113173	-0.124390	-0.346288	H	-2.461829	-3.341416	0.991330
C	2.076701	-0.329355	-1.365009	H	-3.069467	-2.372071	-0.355196
O	5.120944	-0.517040	0.151269	C	-0.546524	-4.769788	-0.460896
O	3.143583	-0.999813	-0.805690	H	1.491206	-4.316958	0.137411
O	2.260868	2.875946	0.370895	H	0.901768	-3.343160	-1.206346
H	0.719600	0.232022	1.616345	H	-2.631960	-4.735986	-1.074946
H	3.211771	0.592215	2.560160	H	-1.596199	-3.603808	-1.942531
C	-0.004743	2.298469	-0.350954	H	-0.258876	-5.548890	-1.174702
H	-0.522762	2.603000	0.563247	H	-0.775992	-5.273671	0.488188
H	0.100308	3.191711	-0.982994	O	1.219579	-0.922169	-1.949759
N	-0.731780	1.219684	-1.001210	H	-0.652380	1.233062	-2.010695
C	-2.075463	0.862472	-0.559973				
H	-2.347242	-0.008184	-1.174430				
C	-3.235140	1.874004	-0.779105				
C	-3.328891	2.139611	-2.286345				
H	-4.162674	2.816435	-2.498888				
H	-2.416106	2.613976	-2.664826				
H	-3.496256	1.213145	-2.849612				
C	-3.050877	3.212726	-0.053489				
H	-2.908259	3.072572	1.020804				
H	-2.203862	3.776267	-0.457645				
H	-3.947216	3.824923	-0.205093				
C	-4.535667	1.214537	-0.301787				
H	-5.394365	1.836431	-0.575332				
H	-4.676692	0.229946	-0.766039				
H	-4.539171	1.088598	0.784700				
C	-1.935636	0.341875	0.845487				
N	-2.149742	0.963127	1.988548				
N	-1.422700	-0.872830	1.125289				
N	-1.345383	-0.997967	2.455763				

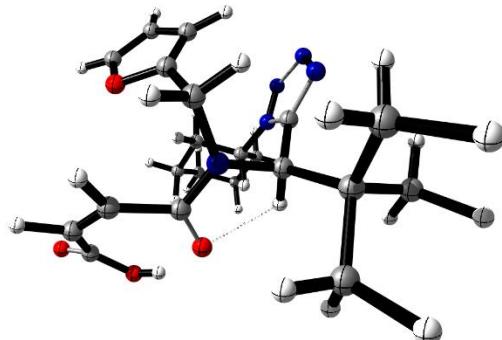


**10m**

E(scf) = -1391.74635456 a.u.

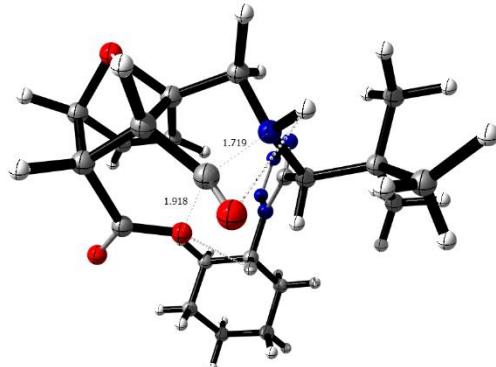
 $\nu_{\min} = 18.22 \text{ cm}^{-1}$ 

C	-1.152986	1.302447	1.643045	H	-1.173448	0.541470	-1.652917
H	-2.207816	1.038860	1.714917	C	0.358414	1.786048	-0.300785
N	-0.827401	1.344749	0.201481	O	0.630961	1.640611	-1.501645
C	-1.741696	0.648569	-0.727219	C	1.289175	2.482455	0.629744
C	-2.999628	1.469589	-1.122545	C	2.613130	2.624741	0.487060
C	-3.887568	1.884201	0.056565	C	3.609924	2.100418	-0.520327
H	-4.217602	1.020378	0.640729	O	3.206252	1.771970	-1.739443
H	-3.376759	2.597403	0.713171	O	4.763641	2.017432	-0.177806
H	-4.777706	2.389816	-0.333067	H	0.854827	2.900502	1.530758
C	-2.507531	2.731584	-1.842618	H	3.136672	3.146838	1.282739
H	-1.894474	3.353466	-1.181675	H	-1.044316	2.302936	2.071523
H	-1.907700	2.482617	-2.724318	C	-0.397446	0.289800	2.439005
H	-3.364659	3.330813	-2.166162	C	-0.744842	-0.924178	2.945560
C	-3.820730	0.618773	-2.100811	O	0.896028	0.572865	2.753271
H	-4.267328	-0.245637	-1.602313	C	0.420034	-1.429505	3.607908
H	-4.628489	1.224613	-2.523741	H	-1.708526	-1.405328	2.850325
H	-3.201424	0.262616	-2.932917	C	1.379299	-0.482953	3.454337
C	-1.987594	-0.736498	-0.204168	H	0.521837	-2.372492	4.123849
N	-3.008584	-1.176888	0.504000	H	2.407874	-0.403527	3.770423
N	-2.736377	-2.464187	0.792311	H	2.220184	1.843924	-1.811379
N	-1.599252	-2.813508	0.300345				
N	-1.108273	-1.748593	-0.340062				
C	0.218502	-1.777844	-0.970352				
C	1.324668	-1.624504	0.075917				
C	0.394744	-3.053043	-1.794767				
H	0.252782	-0.909563	-1.639556				
C	2.691560	-1.620296	-0.612357				
H	1.247015	-2.455698	0.789186				
H	1.178566	-0.698951	0.644083				
C	1.767021	-3.046434	-2.474191				
H	0.308232	-3.917161	-1.125912				
H	-0.411321	-3.130140	-2.532484				
C	2.892783	-2.885134	-1.449388				
H	3.481515	-1.521316	0.139179				
H	2.765055	-0.736589	-1.261234				
H	1.895733	-3.971212	-3.045668				
H	1.813262	-2.218349	-3.194597				
H	3.862824	-2.852530	-1.955503				
H	2.903967	-3.761220	-0.786665				



**TS<sub>[9m<sup>(endo)</sup> → 8m]</sub>**  
E(scf) = -1391.65314337 a.u.  
v<sub>min</sub> = -186.89 cm<sup>-1</sup>

C	2.725683	-0.682696	-0.873244	N	-1.023131	1.126424	3.010676
C	2.595661	-0.339586	0.650696	C	-2.226325	-0.478974	0.133437
C	3.112652	-2.385998	0.697337	C	-2.119239	-1.943228	0.556869
C	2.566678	-2.168448	-0.812897	C	-3.682797	-0.043075	-0.017798
H	3.718078	-0.335916	-1.174036	H	-1.693407	-0.370252	-0.814098
H	3.117433	-2.752553	-1.550130	C	-2.781081	-2.814773	-0.509986
C	1.502872	-1.046953	1.455280	H	-2.619046	-2.069380	1.525432
C	1.875208	-2.320146	1.556241	H	-1.067894	-2.220934	0.664993
H	3.821372	-3.198629	0.833802	C	-4.368793	-0.924717	-1.067018
C	1.028425	-2.364866	-0.953604	H	-4.182472	-0.146479	0.953941
C	1.686896	0.066310	-1.609916	H	-3.735237	1.014980	-0.302262
O	0.521355	-3.467680	-0.870370	C	-4.243247	-2.411180	-0.718692
O	0.377492	-1.236346	-1.092135	H	-2.705915	-3.866659	-0.218645
O	3.741734	-1.112809	1.026392	H	-2.211590	-2.712269	-1.442603
H	0.630325	-0.579085	1.883161	H	-5.421330	-0.636742	-1.158700
H	1.355186	-3.151799	2.011734	H	-3.902870	-0.743277	-2.045398
C	2.448822	1.180448	0.653897	H	-4.700079	-3.018116	-1.507721
H	2.028837	1.596443	1.568170	H	-4.806973	-2.610320	0.203427
H	3.382066	1.686183	0.394607	O	1.490709	0.416064	-2.732760
N	1.488120	1.374363	-0.512808	H	1.882575	2.100177	-1.113770
C	0.040359	1.761208	-0.358609				
H	-0.459474	1.226540	-1.171026				
C	-0.156053	3.285404	-0.613609				
C	0.190878	3.584005	-2.100124				
H	0.755907	4.557859	-2.190688				
H	0.803004	2.763175	-2.579914				
H	-0.757890	3.664807	-2.709832				
C	0.726298	4.129373	0.320150				
H	0.523069	3.908864	1.370375				
H	1.797982	3.966674	0.129910				
H	0.526378	5.188796	0.135737				
C	-1.629945	3.626757	-0.367091				
H	-1.817347	4.665298	-0.657483				
H	-2.287303	2.983605	-0.965981				
H	-1.899605	3.517375	0.690953				
C	-0.545502	1.302585	0.935916				
N	-0.233956	1.771536	2.131741				
N	-1.520153	0.386379	1.093597				
N	-1.797852	0.299742	2.397315				

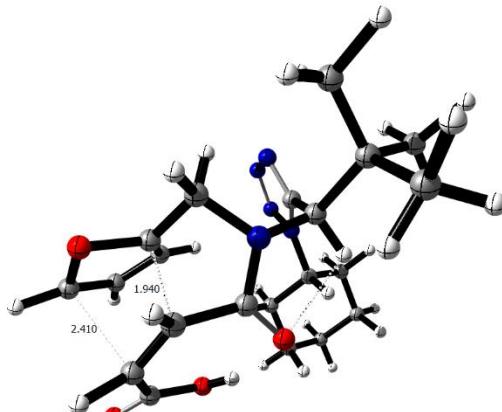


**TS<sub>[10m → 8m<sup>(endo)</sup>]</sub>**

E(scf) = -1391.69436746 a.u.

ν<sub>min</sub> = -456.46 cm<sup>-1</sup>

C	-2.350169	-0.862743	-1.077408	N	1.784005	0.464221	1.049700
C	-2.031443	-1.473017	0.736313	N	1.925371	0.616504	2.373215
C	-4.004715	-0.757835	1.170187	N	1.842355	-0.554070	2.898334
C	-3.447134	-0.008287	-1.051384	C	1.803971	1.636808	0.165795
H	-2.591309	-1.855440	-1.458842	C	0.640182	2.572417	0.492295
H	-4.404467	-0.400605	-1.373727	C	3.148829	2.358368	0.250129
C	-1.861218	-0.299106	1.505762	H	1.655400	1.251704	-0.847638
C	-3.135009	0.186049	1.727982	C	0.644209	3.752940	-0.479061
H	-5.081245	-0.835211	1.211133	H	0.752340	2.925320	1.525454
C	-3.463308	1.468016	-0.856800	H	-0.308515	2.031349	0.421334
C	-0.884718	-0.601257	-1.248952	C	3.152094	3.552928	-0.708549
O	-4.473115	2.062708	-0.568846	H	3.299888	2.698085	1.282158
O	-2.292550	2.121750	-0.977197	H	3.959803	1.660443	0.011760
O	-3.330371	-1.888276	0.870332	C	1.980108	4.498922	-0.428606
H	-0.915284	0.182611	1.722195	H	-0.190194	4.420834	-0.246694
H	-3.430369	1.139392	2.142463	H	0.469658	3.375657	-1.496671
C	-0.922073	-2.402868	0.318105	H	4.105186	4.085465	-0.628721
H	-0.270775	-2.677910	1.151354	H	3.079271	3.185233	-1.741473
H	-1.330529	-3.311481	-0.138102	H	1.983384	5.324493	-1.147945
N	-0.153298	-1.595785	-0.650805	H	2.106863	4.943096	0.568046
H	-1.621280	1.579156	-1.444583				
O	-0.381719	0.358146	-1.830265				
C	1.299937	-1.438320	-0.556753				
H	1.537672	-0.680253	-1.306725				
C	2.122481	-2.689725	-0.951394				
C	1.824908	-2.991442	-2.441132				
H	2.673915	-2.640963	-3.098186				
H	1.684855	-4.099241	-2.607746				
H	0.880575	-2.469395	-2.782465				
C	1.805471	-3.925227	-0.094388				
H	1.925317	-3.720505	0.971382				
H	0.792257	-4.295953	-0.279721				
H	2.495794	-4.727089	-0.373111				
C	3.604945	-2.335900	-0.778417				
H	4.225098	-3.145687	-1.171509				
H	3.858850	-1.420062	-1.323218				
H	3.866142	-2.193725	0.278326				
C	1.620733	-0.849265	0.791484				
N	1.648031	-1.489822	1.946419				

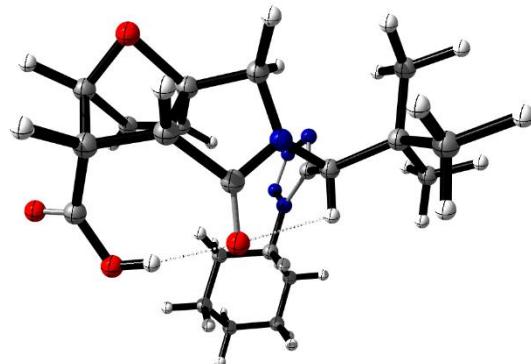


**8m<sup>(endo)</sup>**

E(scf) = -1391.74032208 a.u.

ν<sub>min</sub> = 26.56 cm<sup>-1</sup>

C	1.875035	1.531267	-0.879341	N	-1.553432	-0.978195	1.031308
C	1.503095	2.037272	0.540563	N	-1.631760	-1.184968	2.351728
C	3.559251	1.640085	0.781974	N	-1.972329	-0.067559	2.889505
C	3.310758	1.036450	-0.674764	C	-1.142422	-2.070962	0.138980
H	1.911613	2.428762	-1.509632	C	0.302704	-2.480582	0.423691
H	3.975457	1.520618	-1.396658	C	-2.100015	-3.256014	0.262760
C	1.572158	0.885874	1.536176	H	-1.187783	-1.666070	-0.876828
C	2.872348	0.662102	1.719033	C	0.724580	-3.581827	-0.549482
H	4.585040	1.930358	0.992513	H	0.368342	-2.836593	1.459998
C	3.665287	-0.446314	-0.699772	H	0.964648	-1.613683	0.327351
C	0.594775	0.829610	-1.236940	C	-1.670242	-4.370892	-0.696011
O	4.639761	-0.841484	-0.111788	H	-2.078156	-3.615739	1.298484
O	2.906554	-1.274958	-1.419928	H	-3.124195	-2.928078	0.050940
O	2.675683	2.777787	0.831097	C	-0.215976	-4.785635	-0.454530
H	0.717738	0.371948	1.966320	H	1.760230	-3.871050	-0.349373
H	3.366690	-0.106674	2.297173	H	0.706502	-3.177275	-1.571183
C	0.113716	2.599533	0.296305	H	-2.340487	-5.229258	-0.584449
H	-0.518479	2.646476	1.186096	H	-1.777354	-4.017303	-1.730912
H	0.148723	3.578838	-0.193879	H	0.079529	-5.556635	-1.173799
N	-0.400863	1.556934	-0.633546	H	-0.130182	-5.232278	0.545422
H	2.089812	-0.858583	-1.777689				
O	0.430855	-0.183566	-1.911627				
C	-1.749971	0.992573	-0.545855				
H	-1.764452	0.215384	-1.315848				
C	-2.900667	1.962596	-0.909487				
C	-2.689372	2.395193	-2.364587				
H	-3.491897	3.072004	-2.674511				
H	-1.736662	2.921599	-2.484862				
H	-2.690075	1.533704	-3.042344				
C	-2.981869	3.207115	-0.017272				
H	-3.027615	2.944640	1.042422				
H	-2.134549	3.879523	-0.182818				
H	-3.888004	3.766284	-0.274359				
C	-4.211600	1.173857	-0.792053				
H	-5.041421	1.773471	-1.179319				
H	-4.171852	0.243218	-1.371744				
H	-4.433702	0.923891	0.250082				
C	-1.864385	0.312165	0.792241				
N	-2.122101	0.887428	1.952662				

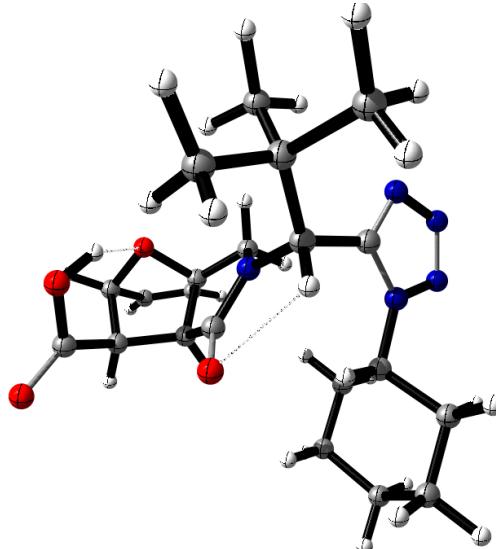


**8m<sup>(exo)</sup>** (*involved in path i*)

E(scf) = -1391.75478918 a.u.

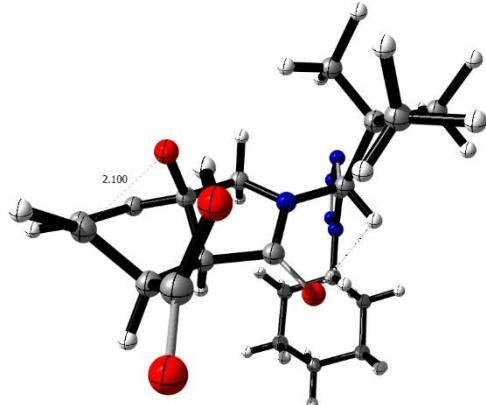
v<sub>min</sub> = 25.25 cm<sup>-1</sup>

C	3.168679	-1.470129	-0.110345	N	-3.364318	1.707571	1.981373
C	1.695368	-1.207545	0.293831	N	-3.581818	0.535483	1.498682
C	3.894684	-0.695497	1.052519	C	-2.582494	-0.925487	-0.193159
C	3.613339	-1.399750	2.369241	C	-1.983845	-2.001988	0.714042
C	1.855598	-0.264423	1.524335	C	-3.932392	-1.366731	-0.756553
O	3.043115	0.453587	1.152195	H	-1.889726	-0.750132	-1.024864
C	0.649625	0.647033	1.506528	C	-1.784958	-3.291332	-0.085014
H	-0.174605	0.229434	2.102191	H	-2.666737	-2.167963	1.557301
N	0.315965	0.680084	0.079441	H	-1.033503	-1.646261	1.132111
H	3.217496	0.829305	-0.703633	C	-3.752829	-2.668118	-1.545531
C	3.556614	-0.891508	-1.470572	H	-4.631202	-1.514997	0.075322
C	0.794516	-0.396537	-0.631392	H	-4.342976	-0.575797	-1.392968
O	3.498368	0.450170	-1.560168	C	-3.111969	-3.762611	-0.687243
H	3.413017	-2.531128	-0.134072	H	-1.358040	-4.068961	0.557253
H	1.173626	-2.139639	0.530691	H	-1.061122	-3.101026	-0.890763
O	3.925372	-1.570431	-2.386392	H	-4.721668	-3.003189	-1.928797
O	0.494842	-0.673335	-1.775837	H	-3.115408	-2.473856	-2.418796
C	2.350960	-1.102547	2.682235	H	-2.954602	-4.666101	-1.285148
H	1.746349	-1.467824	3.502930	H	-3.798638	-4.032891	0.126643
H	4.298863	-2.063388	2.880143	H	4.922224	-0.398672	0.843720
H	0.883845	1.639556	1.893507				
C	-0.729334	1.538627	-0.479688				
H	-1.003712	1.054629	-1.425009				
C	-0.253508	2.963050	-0.861615				
C	0.727139	2.812851	-2.031295				
H	1.569742	2.160986	-1.780685				
H	0.233005	2.386407	-2.911078				
H	1.129243	3.793078	-2.307304				
C	0.444628	3.685363	0.295259				
H	-0.185985	3.721196	1.188763				
H	1.400097	3.205475	0.537441				
H	0.667510	4.714937	-0.004420				
C	-1.466624	3.777562	-1.329004				
H	-1.123712	4.717059	-1.774525				
H	-2.034401	3.235605	-2.095456				
H	-2.137112	4.013855	-0.499208				
C	-1.916662	1.452112	0.438192				
N	-2.686658	0.347641	0.522405				
N	-2.330976	2.304362	1.352628				



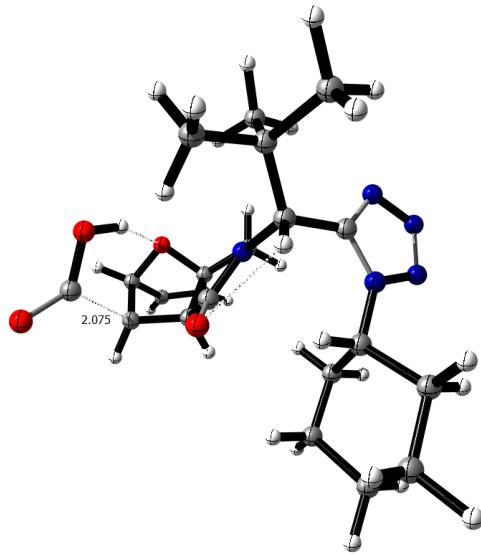
**TS<sub>[8m<sup>(exo)</sup> → 12m]</sub>**  
 E(scf) = -1391.67769142 a.u.  
 ν<sub>min</sub> = -312.39 cm<sup>-1</sup>

C	3.129023	-1.530615	-0.128542	N	-3.455887	1.761825	1.883402
C	1.723473	-1.148682	0.383028	N	-3.655230	0.574485	1.431619
C	4.073156	-1.074286	0.970986	C	-2.599840	-0.937305	-0.177902
C	3.686401	-1.382846	2.360339	C	-2.032523	-1.983408	0.783818
C	1.961560	-0.091785	1.495492	C	-3.930493	-1.396227	-0.772227
O	3.003908	0.731817	1.039485	H	-1.879931	-0.788813	-0.991408
C	0.647176	0.681743	1.522581	C	-1.813525	-3.301667	0.039229
H	-0.113947	0.183690	2.141788	H	-2.740595	-2.117282	1.611877
N	0.274516	0.653626	0.104769	H	-1.094018	-1.614200	1.216083
H	3.200094	0.772504	-0.638646	C	-3.726629	-2.724600	-1.508621
C	3.516792	-0.908123	-1.486074	H	-4.659072	-1.514246	0.038557
C	0.780203	-0.424863	-0.570876	H	-4.316212	-0.627680	-1.450203
O	3.451547	0.417944	-1.534930	C	-3.121890	-3.789819	-0.589245
H	3.232876	-2.613131	-0.257650	H	-1.411938	-4.056511	0.723618
H	1.189944	-2.029579	0.760635	H	-1.062595	-3.143100	-0.748060
O	3.877191	-1.590726	-2.405700	H	-4.681850	-3.070664	-1.915679
O	0.488329	-0.763732	-1.702468	H	-3.055920	-2.562748	-2.363292
C	2.501743	-0.850094	2.691941	H	-2.950053	-4.715783	-1.147529
H	2.006951	-0.962725	3.650915	H	-3.837591	-4.025625	0.210211
H	4.343146	-1.942945	3.016987	H	5.107501	-0.846736	0.719654
H	0.778158	1.699678	1.886877				
C	-0.743216	1.517508	-0.494607				
H	-0.999556	1.023989	-1.438566				
C	-0.226175	2.926023	-0.884717				
C	0.852202	2.738446	-1.985076				
H	1.239119	1.681020	-2.033424				
H	0.422837	2.994167	-3.000169				
H	1.734981	3.421546	-1.794780				
C	0.380457	3.686175	0.302642				
H	-0.310031	3.741618	1.149751				
H	1.324972	3.228374	0.617842				
H	0.613563	4.710976	-0.017236				
C	-1.404333	3.731102	-1.445348				
H	-1.034964	4.669772	-1.867050				
H	-1.905701	3.179768	-2.252947				
H	-2.140790	3.966091	-0.672835				
C	-1.954373	1.459917	0.395810				
N	-2.727042	0.357489	0.493427				
N	-2.402402	2.340658	1.266465				



**TS' [ $(8m^{(exo)} \rightarrow 12m)$ ]**  
E(scf) = -1391.69265687 a.u.  
 $\nu_{\min} = -90.41 \text{ cm}^{-1}$

C	3.037031	-1.761794	-0.019336	N	-3.238319	1.881140	1.993928
C	1.604127	-1.401234	0.385151	N	-3.551945	0.742995	1.488815
C	3.850490	-1.027347	1.072808	C	-2.661102	-0.769998	-0.215929
C	3.557998	-1.660737	2.424809	C	-2.202519	-1.917982	0.684604
C	1.857139	-0.441094	1.582911	C	-4.029972	-1.063262	-0.830167
O	3.082701	0.189760	1.159812	H	-1.927664	-0.650326	-1.021768
C	0.710927	0.547398	1.563679	C	-2.118740	-3.208308	-0.133594
H	-0.132994	0.186598	2.166947	H	-2.920645	-2.025216	1.507735
N	0.379149	0.589595	0.135241	H	-1.231072	-1.669919	1.131290
H	3.215087	0.670155	-0.617481	C	-3.960388	-2.361363	-1.641172
C	3.506436	-0.780433	-1.786147	H	-4.768244	-1.153707	-0.024579
C	0.767432	-0.539219	-0.551964	H	-4.334560	-0.221738	-1.461198
O	3.468288	0.521254	-1.558496	C	-3.469233	-3.530641	-0.777874
H	3.264036	-2.804298	-0.220384	H	-1.797101	-4.037062	0.510798
H	1.011387	-2.283739	0.657166	H	-1.353873	-3.083966	-0.913339
O	3.794677	-1.338645	-2.781976	H	-4.944599	-2.584578	-2.064891
O	0.458475	-0.800671	-1.699328	H	-3.273260	-2.221050	-2.486486
C	2.327400	-1.266532	2.758421	H	-3.392141	-4.438084	-1.385448
H	1.717401	-1.559729	3.607024	H	-4.207132	-3.729432	0.009945
H	4.208536	-2.352672	2.944194	H	4.890849	-0.811892	0.833023
H	1.011673	1.526024	1.942436				
C	-0.592255	1.527545	-0.433724				
H	-0.883113	1.071666	-1.390082				
C	-0.000927	2.920570	-0.795870				
C	1.004077	2.711739	-1.955723				
H	1.381574	1.648312	-1.988019				
H	0.511718	2.936349	-2.947022				
H	1.892497	3.397282	-1.835618				
C	0.706955	3.580549	0.397921				
H	0.062116	3.630897	1.278491				
H	1.633360	3.050498	0.644293				
H	0.984411	4.602600	0.120496				
C	-1.143538	3.825802	-1.267222				
H	-0.722758	4.741706	-1.699343				
H	-1.735167	3.335759	-2.055440				
H	-1.814609	4.103652	-0.446929				
C	-1.796683	1.524638	0.462293				
N	-2.659313	0.493058	0.518759				
N	-2.144825	2.393575	1.391947				

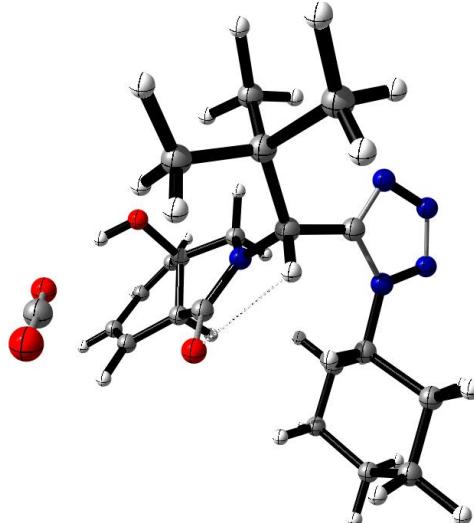


**12m**

E(scf) = -1391.76953014 a.u.

 $\nu_{\min} = 28.97 \text{ cm}^{-1}$ 

C	-2.796823	-2.293541	0.062356	C	2.620807	-0.710995	0.266130
C	-1.671358	-1.434437	-0.409339	C	2.245953	-1.931731	-0.575923
C	-3.616943	-2.763330	-0.891706	C	3.957686	-0.918024	0.977805
C	-3.428104	-2.386452	-2.306160	H	1.838181	-0.550939	1.018015
C	-2.081115	-0.507287	-1.553993	C	2.154992	-3.169081	0.319230
O	-3.031077	0.460426	-1.125292	H	3.011860	-2.069140	-1.350115
C	-0.790390	0.291205	-1.735781	H	1.295198	-1.745723	-1.089524
H	-0.036551	-0.274218	-2.301921	C	3.880858	-2.164207	1.865151
N	-0.383704	0.468342	-0.334613	H	4.743433	-1.035129	0.222265
C	-3.046282	0.295739	2.745281	H	4.202260	-0.029228	1.568907
C	-0.893515	-0.493615	0.490953	C	3.476038	-3.401107	1.058046
O	-3.612016	0.017719	1.763550	H	1.889828	-4.045780	-0.280486
H	-0.909447	-2.117661	-0.833416	H	1.346587	-3.021136	1.049901
O	-2.527089	0.585965	3.741158	H	4.846077	-2.326395	2.355213
O	-0.695107	-0.587703	1.693023	H	3.143510	-1.996000	2.661822
C	-2.663133	-1.342581	-2.666830	H	3.394857	-4.271952	1.716738
H	-2.580094	-1.020548	-3.700891	H	4.262040	-3.625950	0.324216
H	-3.961996	-2.959342	-3.059225	H	-4.426998	-3.443271	-0.645668
H	-0.960996	1.247996	-2.227190	H	-3.760726	-0.010063	-0.689026
C	0.484060	1.529065	0.158815	H	-2.886211	-2.562037	1.109770
H	0.742253	1.211396	1.177265				
C	-0.197882	2.913268	0.325257				
C	-1.358181	2.726262	1.311112				
H	-2.109298	2.048921	0.888030				
H	-1.010994	2.322788	2.269556				
H	-1.840694	3.691160	1.499529				
C	-0.755702	3.498584	-0.978687				
H	-0.003191	3.515643	-1.771977				
H	-1.639180	2.943459	-1.309909				
H	-1.076130	4.529928	-0.793152				
C	0.835600	3.875845	0.924504				
H	0.345702	4.817445	1.192891				
H	1.282011	3.461171	1.836706				
H	1.634667	4.096711	0.211932				
C	1.748209	1.500993	-0.654911				
N	2.642742	0.495731	-0.561459				
N	2.165406	2.326391	-1.592452				
N	3.321341	1.811383	-2.059036				
N	3.613884	0.715181	-1.454958				

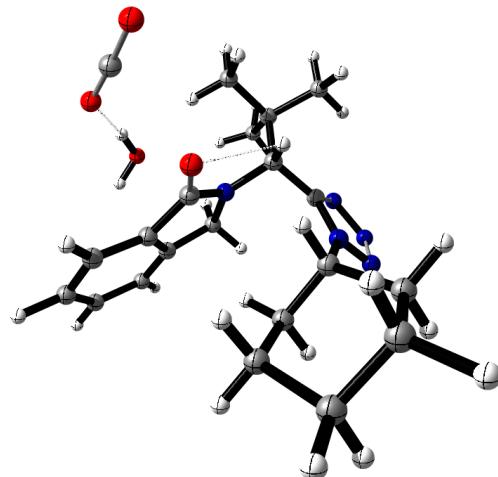


**13m**

E(scf) = -1391.81599277 a.u.

 $\nu_{\min} = 31.02 \text{ cm}^{-1}$ 

C	2.087935	2.736248	0.002474	C	-2.172487	1.726387	-0.387694
C	1.485895	1.548077	-0.385748	C	-3.818489	0.644125	1.187786
C	2.544017	3.585715	-1.002530	H	-1.696893	0.304847	1.153955
C	2.390148	3.238467	-2.348799	C	-2.052382	2.930248	0.548081
C	1.326079	1.194954	-1.721910	H	-2.974302	1.883151	-1.121270
O	3.592406	-0.715298	-1.109123	H	-1.241797	1.577278	-0.945902
C	0.672005	-0.159693	-1.804458	C	-3.720146	1.859211	2.115630
H	-0.291000	-0.132158	-2.332702	H	-4.628508	0.781288	0.461920
N	0.480059	-0.499404	-0.397357	H	-4.038707	-0.266262	1.755203
C	3.109901	-0.227756	2.732843	C	-3.345617	3.127986	1.343475
C	0.910898	0.474054	0.461035	H	-1.810580	3.828437	-0.029131
O	3.666980	0.121305	1.766696	H	-1.214143	2.757245	1.238815
O	2.616523	-0.588264	3.716711	H	-4.671003	1.998350	2.639910
O	0.797714	0.452468	1.681830	H	-2.958645	1.666457	2.883532
C	1.780934	2.039897	-2.726020	H	-3.243740	3.971937	2.033770
H	1.669367	1.782095	-3.775123	H	-4.158210	3.379065	0.648021
H	2.752425	3.915598	-3.116257	H	3.024891	4.523697	-0.744216
H	1.325067	-0.884163	-2.297908	H	3.657214	0.180387	-1.469963
C	-0.274501	-1.651720	0.084207	H	2.197167	2.975701	1.055922
H	-0.475378	-1.417596	1.137529	H	3.848800	-0.607858	-0.181559
C	0.513903	-2.984998	0.097326				
C	1.693029	-2.795545	1.060004				
H	2.342414	-1.989247	0.703246				
H	1.351696	-2.556065	2.074196				
H	2.288171	-3.713675	1.103549				
C	1.059166	-3.375211	-1.281412				
H	0.276960	-3.351024	-2.045850				
H	1.889577	-2.722543	-1.570459				
H	1.452254	-4.396877	-1.233924				
C	-0.406785	-4.088285	0.633460				
H	0.180328	-4.993378	0.820206				
H	-0.871150	-3.791739	1.582206				
H	-1.196148	-4.331487	-0.081787				
C	-1.598073	-1.662752	-0.631449				
N	-2.532730	-0.709406	-0.431972				
N	-2.040058	-2.469882	-1.573456				
N	-3.250733	-1.998002	-1.935669				
N	-3.552521	-0.943201	-1.265395				
C	-2.502638	0.474942	0.429048				

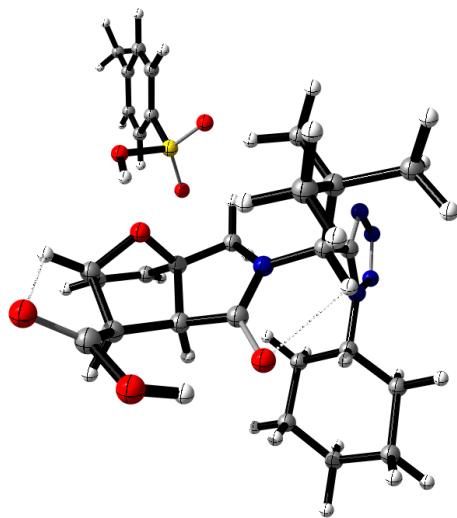


**8m<sup>(exo)</sup> +PTSA**

E(scf) = -2286.89695331 a.u.

v<sub>min</sub> = -5.77 cm<sup>-1</sup>

C	-1.047998	3.487863	-0.450652	C	-4.000108	-1.507247	-0.858224
C	-1.458086	2.009164	-0.694841	C	-3.465860	-0.893558	-2.154145
C	0.504322	3.336050	-0.465707	C	-5.337348	-2.210243	-1.092116
C	0.958785	2.927762	-1.858801	H	-4.146242	-0.704709	-0.124698
C	-0.075719	1.284142	-0.706914	C	-4.476852	0.118585	-2.698174
O	0.630056	2.092847	0.255650	H	-3.296846	-1.699781	-2.879574
C	-0.330453	-0.112321	-0.176763	H	-2.494665	-0.418501	-1.968816
H	-0.495547	-0.825940	-0.994541	C	-6.353332	-1.209461	-1.652023
N	-1.553027	0.077913	0.616146	H	-5.183838	-3.034712	-1.798028
C	-1.472174	4.235949	0.827532	H	-5.692951	-2.646141	-0.152713
C	-2.230115	1.212621	0.338666	C	-5.837283	-0.544607	-2.931073
O	-2.698111	4.043309	1.300568	H	-4.101046	0.560915	-3.626846
H	-1.389673	4.116350	-1.279354	H	-4.588002	0.935711	-1.970164
H	-1.994041	1.896570	-1.643512	H	-7.303633	-1.717897	-1.842625
O	-0.735176	5.056035	1.311611	H	-6.552179	-0.436409	-0.897261
O	-3.338319	1.508415	0.791058	H	-6.560855	0.192971	-3.292878
C	0.624307	1.644789	-1.999989	H	-5.733920	-1.304628	-3.717262
H	0.733197	0.988652	-2.852916	H	1.024228	4.140890	0.047566
H	1.406107	3.593897	-2.584915	H	-3.127081	3.223948	0.961235
H	0.490706	-0.489144	0.434155	H	2.333391	1.679317	0.264198
C	-2.104848	-0.931392	1.522452	O	3.273174	1.370103	0.130624
H	-3.136567	-0.602072	1.696707	S	3.231856	-0.210844	-0.103457
C	-1.437162	-0.966825	2.921494	O	2.761387	-0.849741	1.115837
C	-1.646742	0.415216	3.554848	O	2.522844	-0.486757	-1.346549
H	-1.145130	1.198419	2.975296	C	4.952719	-0.528786	-0.314694
H	-2.709757	0.670819	3.627772	C	5.492671	-0.537236	-1.595807
H	-1.220685	0.425091	4.563108	C	5.729998	-0.773369	0.812360
C	0.063660	-1.274130	2.881190	C	6.850953	-0.790860	-1.742463
H	0.289311	-2.168199	2.293702	H	4.852189	-0.357092	-2.453028
H	0.638976	-0.433564	2.482418	C	7.085794	-1.023100	0.643125
H	0.418117	-1.442491	3.904133	H	5.271279	-0.776859	1.795995
C	-2.165836	-2.026323	3.758671	C	7.662304	-1.036975	-0.630742
H	-1.818941	-1.971062	4.795408	H	7.289733	-0.802990	-2.736466
H	-3.249672	-1.856328	3.761081	H	7.707542	-1.217610	1.512687
H	-1.968818	-3.034427	3.385143	C	9.125838	-1.347804	-0.805324
C	-2.172082	-2.230066	0.767191	H	9.275849	-2.424456	-0.942458
N	-3.018121	-2.417621	-0.268050	H	9.537057	-0.842696	-1.683140
N	-1.445069	-3.319187	0.896932	H	9.703597	-1.042545	0.070704
N	-1.862367	-4.166549	-0.065086				
N	-2.797680	-3.637486	-0.771319				

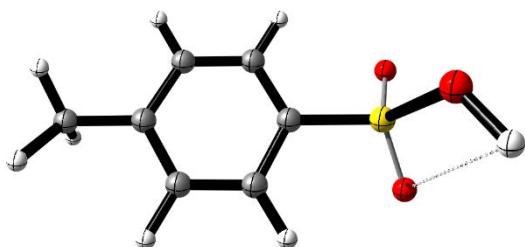


**PTSA**

E(scf) = -895.115442598 a.u.

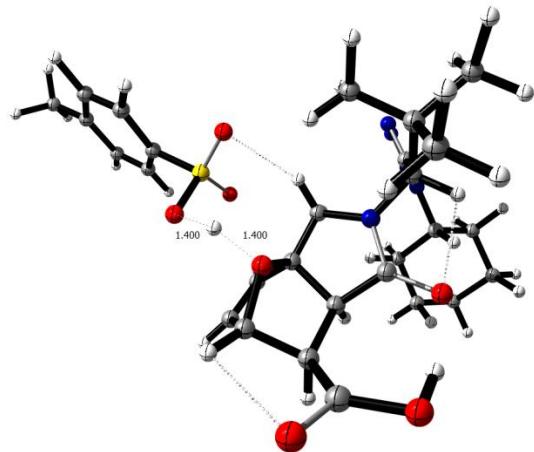
v<sub>min</sub> = 42.35 cm<sup>-1</sup>

H	-2.668017	0.784186	1.680519
O	-2.281960	-0.078395	1.446005
S	-1.891243	-0.017559	-0.128404
O	-2.327708	-1.264427	-0.709087
O	-2.360166	1.269209	-0.610027
C	-0.123483	-0.007557	-0.077221
C	0.549653	1.210084	-0.087346
C	0.557313	-1.219095	-0.023684
C	1.937719	1.204912	-0.033312
H	-0.010090	2.137630	-0.153056
C	1.945880	-1.201680	0.032173
H	0.003043	-2.151976	-0.036583
C	2.652471	0.004274	0.027710
H	2.478469	2.147467	-0.044063
H	2.491855	-2.140011	0.075193
C	4.158670	0.014676	0.054216
H	4.560865	0.122714	-0.959064
H	4.537710	0.850002	0.649309
H	4.555380	-0.913844	0.471868



**TS<sub>[8m<sup>(exo)</sup> +PTSA → 11m]</sub>**  
E(scf) = -2286.85771942 a.u.  
v<sub>min</sub> = -1505.27 cm<sup>-1</sup>

C	-0.994023	3.469403	-0.487347	N	-2.816847	-3.642980	-0.728384
C	-1.391566	1.980481	-0.707687	C	-3.974216	-1.492251	-0.870813
C	0.554675	3.339095	-0.476418	C	-3.402081	-0.904917	-2.162763
C	1.048716	2.877074	-1.833753	C	-5.317075	-2.177558	-1.124597
C	-0.019273	1.248606	-0.679227	H	-4.123981	-0.678402	-0.150555
O	0.643734	2.107767	0.306534	C	-4.384268	0.115826	-2.742399
C	-0.286966	-0.133213	-0.121381	H	-3.230647	-1.723394	-2.873620
H	-0.428226	-0.856362	-0.934914	H	-2.426310	-0.445098	-1.962446
N	-1.530045	0.075178	0.634961	C	-6.304432	-1.169070	-1.720384
C	-1.449471	4.235542	0.771382	H	-5.160825	-3.014266	-1.815266
C	-2.193964	1.207554	0.323051	H	-5.699606	-2.594844	-0.187397
O	-2.695267	4.070354	1.195364	C	-5.749587	-0.529727	-2.996252
H	-1.322008	4.077170	-1.336294	H	-3.981886	0.539895	-3.668472
H	-1.897350	1.844724	-1.669409	H	-4.499422	0.944108	-2.027533
O	-0.711988	5.042643	1.275327	H	-7.257907	-1.665505	-1.925881
O	-3.309242	1.523940	0.741187	H	-6.508476	-0.383048	-0.980493
C	0.726122	1.590199	-1.947716	H	-6.453334	0.213885	-3.383702
H	0.896181	0.898547	-2.760510	H	-5.640732	-1.301524	-3.769983
H	1.544953	3.515867	-2.551742	H	1.064482	4.151296	0.034310
H	0.520389	-0.504952	0.511761	H	-3.117299	3.242397	0.866293
C	-2.109610	-0.919548	1.542160	H	1.969980	1.738437	0.560829
H	-3.137815	-0.570943	1.698541	O	3.192620	1.413380	-0.038745
C	-1.463327	-0.953784	2.951812	S	3.186662	-0.138248	-0.108575
C	-1.634676	0.445126	3.558592	O	2.735341	-0.675859	1.177129
H	-1.090865	1.199690	2.978875	O	2.462827	-0.593077	-1.298529
H	-2.688673	0.741968	3.602826	C	4.901071	-0.526222	-0.318611
H	-1.231415	0.456057	4.575955	C	5.410843	-0.713016	-1.596864
C	0.025239	-1.320785	2.948105	C	5.708469	-0.634073	0.810124
H	0.224573	-2.236372	2.385213	C	6.763769	-1.005345	-1.743121
H	0.649274	-0.517700	2.545850	H	4.749203	-0.648791	-2.454371
H	0.349379	-1.482411	3.982133	C	7.055388	-0.927181	0.644244
C	-2.246395	-1.971597	3.792220	H	5.273200	-0.510056	1.796333
H	-1.912820	-1.915531	4.833181	C	7.601517	-1.111189	-0.629635
H	-3.322637	-1.759557	3.775582	H	7.175034	-1.160475	-2.736873
H	-2.082776	-2.991780	3.435846	H	7.696166	-1.022832	1.517241
C	-2.188475	-2.224742	0.798827	C	9.069935	-1.403708	-0.794181
N	-3.020094	-2.410714	-0.248496	H	9.277153	-1.856406	-1.772457
N	-1.488405	-3.327266	0.959095	H	9.660527	-0.478858	-0.720889
N	-1.906346	-4.180616	0.003172	H	9.427852	-2.087259	-0.013674

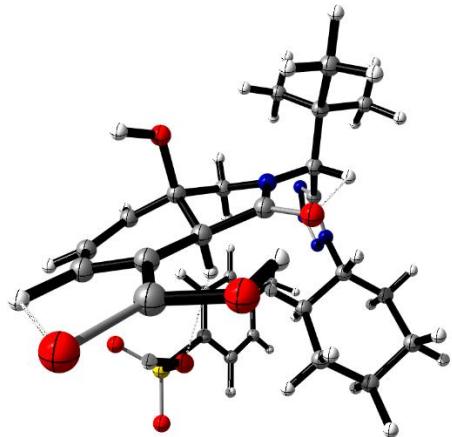


**11m+PTSA**

E(scf) = -2286.89941183 a.u.

 $\nu_{\min} = 16.14 \text{ cm}^{-1}$ 

C	-1.037986	-3.267664	-0.333952	N	1.734635	3.118057	0.256515
C	-0.139210	-2.127065	0.061094	C	1.222470	1.686304	-1.655622
C	-1.948750	-3.613044	0.604210	C	-0.261542	1.455932	-1.372201
C	-1.988743	-2.987579	1.932617	C	1.428612	2.803881	-2.676688
C	0.277615	-2.186756	1.537427	H	1.657533	0.758823	-2.046265
O	1.143319	-3.282268	1.795777	C	-1.001728	1.103918	-2.661472
C	1.171875	-0.953462	1.621941	H	-0.671868	2.373526	-0.931978
H	0.583348	-0.027488	1.690089	H	-0.377795	0.666579	-0.620756
N	1.867220	-1.028059	0.331916	C	0.687132	2.455433	-3.971428
C	-1.144919	-3.946006	-1.685853	H	1.039019	3.738720	-2.256159
C	1.157384	-1.701343	-0.603554	H	2.498843	2.946990	-2.860686
O	-0.323950	-3.561012	-2.651379	C	-0.800336	2.198744	-3.712439
H	-3.064353	-1.649616	-0.444129	H	-2.064932	0.960016	-2.445656
H	-0.772397	-1.222544	-0.019654	H	-0.623833	0.144833	-3.044341
O	-1.976514	-4.801734	-1.866073	H	0.817146	3.263874	-4.697716
O	1.486070	-1.828854	-1.782413	H	1.136757	1.556032	-4.414031
C	-0.951451	-2.272342	2.399982	H	-1.303886	1.925815	-4.645266
H	-0.936318	-1.878966	3.413184	H	-1.269066	3.126565	-3.355467
H	-2.873726	-3.144234	2.540487	H	-2.676908	-4.379623	0.352180
H	1.867622	-1.003336	2.458295	H	0.355299	-2.892648	-2.379671
C	3.047147	-0.237959	-0.008568	O	-2.946862	-0.684534	-0.569505
H	3.116658	-0.299903	-1.100258	S	-3.952156	0.084640	0.456161
C	4.383678	-0.813802	0.523524	O	-5.100956	0.551824	-0.285281
C	4.572053	-2.184227	-0.139602	O	-4.108393	-0.795576	1.600990
H	3.757103	-2.863297	0.133688	H	0.624091	-4.097044	1.703771
H	4.602689	-2.103426	-1.231933	C	-2.933185	1.465625	0.869858
H	5.512736	-2.631229	0.197599	C	-1.883126	1.285141	1.765397
C	4.418847	-0.995159	2.045729	C	-3.196521	2.703323	0.292365
H	4.147160	-0.075707	2.571840	C	-1.060958	2.365619	2.063659
H	3.759036	-1.811889	2.357006	H	-1.730051	0.309547	2.220398
H	5.435471	-1.272023	2.345207	C	-2.377317	3.777945	0.623168
C	5.506246	0.135187	0.087436	H	-4.030925	2.811001	-0.393307
H	6.477598	-0.319218	0.306791	C	-1.300289	3.627525	1.503920
H	5.466478	0.329842	-0.991420	H	-0.225125	2.241772	2.748681
H	5.448972	1.090688	0.616814	H	-2.572547	4.753774	0.186270
C	2.727571	1.186760	0.351349	C	-0.436963	4.808094	1.858856
N	1.929471	1.971596	-0.401222	H	-0.976681	5.482931	2.532570
N	3.016272	1.842529	1.457819	H	0.488396	4.492471	2.344594
N	2.391388	3.031638	1.359903	H	-0.167309	5.372898	0.962289

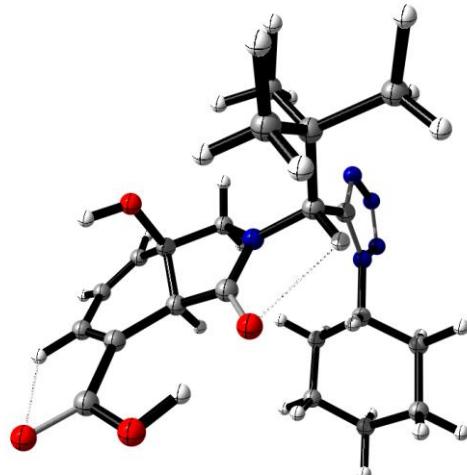


**11m**

E(scf) = -1391.75992987 a.u.

 $\nu_{\min} = 19.37 \text{ cm}^{-1}$ 

C	3.424588	-0.581638	0.055855	C	-0.778179	-3.506760	0.426432
C	1.997936	-0.210732	0.377899	H	-1.960976	-2.457229	1.919779
C	4.290314	-0.427271	1.078954	H	-0.550775	-1.552266	1.363968
C	3.888395	0.133572	2.375158	C	-2.819552	-3.706166	-1.048751
C	1.930441	1.040703	1.267114	H	-4.019861	-2.637608	0.413448
C	0.424003	1.259389	1.356271	H	-3.999004	-1.877957	-1.180372
H	-0.043913	0.586388	2.088154	C	-1.901552	-4.427331	-0.057925
N	0.018375	0.915954	-0.011615	H	-0.149967	-4.021064	1.160839
C	0.888221	0.080024	-0.622293	H	-0.129273	-3.240596	-0.420619
H	1.596849	-1.042352	0.989454	H	-3.643937	-4.359243	-1.351599
O	0.731763	-0.407169	-1.741391	H	-2.253203	-3.467217	-1.959198
C	2.737118	0.810817	2.516744	H	-1.480640	-5.327073	-0.517849
H	2.457133	1.293246	3.448793	H	-2.492230	-4.755998	0.807911
H	4.571733	0.019584	3.211334	H	5.314431	-0.756966	0.932210
H	0.170712	2.289346	1.603078	O	2.413544	2.184021	0.574799
C	-1.225276	1.345922	-0.645969	H	3.365142	2.059883	0.427953
H	-1.328222	0.691096	-1.519849	C	3.953914	-1.249295	-1.195044
C	-1.188863	2.789351	-1.212874	O	5.123015	-1.535370	-1.281563
C	-0.077757	2.830586	-2.269962	O	3.100680	-1.528416	-2.171835
H	0.900992	2.643188	-1.815311	H	2.189129	-1.166920	-2.039125
H	-0.241011	2.087653	-3.058482				
H	-0.048462	3.822380	-2.732907				
C	-0.901243	3.863837	-0.156957				
H	-1.588182	3.795064	0.691071				
H	0.134589	3.803642	0.193003				
H	-1.027467	4.850323	-0.616140				
C	-2.543846	3.064379	-1.877784				
H	-2.497536	4.013908	-2.420435				
H	-2.797837	2.280385	-2.601838				
H	-3.346309	3.132178	-1.138322				
C	-2.345307	1.017875	0.300720				
N	-2.735937	-0.249343	0.548437				
N	-3.042399	1.816447	1.081817				
N	-3.861444	1.019730	1.797731				
N	-3.683873	-0.216289	1.492338				
C	-2.234990	-1.515246	0.009449				
C	-1.351998	-2.226089	1.036370				
C	-3.382816	-2.413322	-0.450272				
H	-1.618286	-1.251425	-0.858795				

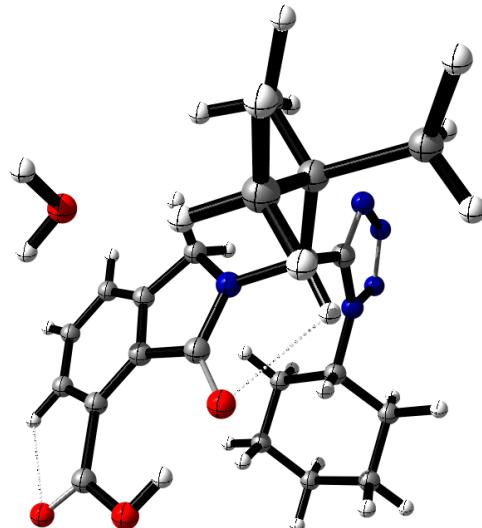


**1m**

E(scf) = -1391.80443795 a.u.

 $\nu_{\min} = 31.89 \text{ cm}^{-1}$ 

C	-3.182884	-0.493573	0.083826	H	0.294369	2.843130	1.841273
C	-1.814874	-0.760094	0.244815	H	-0.327331	1.274314	1.321044
C	-4.011290	-0.766056	1.175367	C	0.440157	4.267218	-1.142382
C	-3.505810	-1.269502	2.373132	H	1.949933	4.105878	0.415479
C	-1.309112	-1.245942	1.452254	H	2.458661	3.443992	-1.141847
C	0.180673	-1.414576	1.357893	C	-0.786101	4.351349	-0.228026
H	0.719617	-0.772986	2.068603	H	-2.054129	3.046865	0.962704
N	0.453247	-0.999129	-0.012327	H	-1.544527	2.351127	-0.574051
C	-0.656488	-0.602087	-0.679042	H	0.757137	5.269324	-1.447831
O	-0.652365	-0.153306	-1.830885	H	0.169823	3.726139	-2.059318
C	-2.142828	-1.511880	2.528137	H	-1.615905	4.831525	-0.756039
H	-1.744931	-1.894851	3.463020	H	-0.546777	4.985082	0.636851
H	-4.185339	-1.465867	3.196496	H	-5.070348	-0.564658	1.058357
H	0.471500	-2.453826	1.522723	O	-0.948512	-3.774280	-0.024697
C	1.789834	-0.806615	-0.574375	H	-1.898646	-3.593356	-0.001895
H	1.615316	-0.227072	-1.489037	C	-3.884546	0.087125	-1.136017
C	2.495343	-2.106142	-1.035307	O	-5.082970	0.228753	-1.120982
C	1.631011	-2.712649	-2.147710	O	-3.160874	0.448767	-2.183141
H	0.630718	-2.952631	-1.772328	H	-0.850592	-4.534818	-0.613420
H	1.525312	-2.023314	-2.992860	H	-2.191841	0.232414	-2.111231
H	2.094812	-3.635017	-2.513807				
C	2.662787	-3.135485	0.088458				
H	3.130696	-2.695634	0.973961				
H	1.698455	-3.578771	0.358015				
H	3.306443	-3.948477	-0.265227				
C	3.868744	-1.727427	-1.604690				
H	4.313316	-2.601060	-2.092288				
H	3.781107	-0.935524	-2.358721				
H	4.548598	-1.388327	-0.819154				
C	2.554244	0.077830	0.373859				
N	2.228993	1.373153	0.569592				
N	3.543693	-0.218453	1.190137				
N	3.815982	0.911302	1.875263				
N	3.032335	1.866512	1.517340				
C	1.138504	2.160113	-0.011255				
C	-0.034629	2.268392	0.965563				
C	1.607033	3.543158	-0.460581				
H	0.808080	1.603161	-0.896176				
C	-1.207353	2.966852	0.273466				

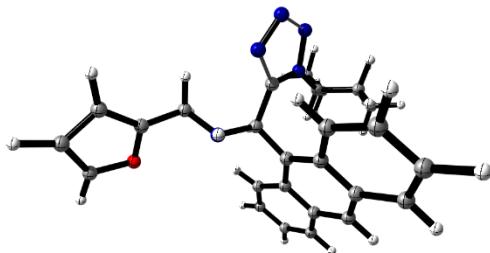


**6j**

E(scf) = -1394.11203789 a.u.

 $\nu_{\min} = 7.97 \text{ cm}^{-1}$ 

C	6.255951	0.523144	-0.883212	C	-0.499368	0.970898	1.632745
C	6.719547	-0.432911	-0.031494	C	-1.076297	3.015014	-0.262832
C	4.535430	-0.763261	-0.434978	C	0.418562	1.965919	-1.905687
O	4.934623	0.337659	-1.139232	C	-1.359990	2.086418	1.974001
C	3.108346	-1.174330	-0.545978	C	-0.196199	0.039645	2.682337
H	2.823903	-1.219944	-1.607413	C	-1.336886	4.044967	-1.220331
N	2.222431	-0.193897	0.100430	C	-1.647295	3.057285	1.011939
C	5.594422	-1.273216	0.261102	C	0.158516	2.982742	-2.788860
H	5.572649	-2.143699	0.903331	H	1.167555	1.227118	-2.170863
H	7.730199	-0.529612	0.341128	C	-1.903985	2.182110	3.293637
H	3.002303	-2.188293	-0.135959	C	-0.725667	0.178315	3.939931
C	0.801242	-0.363438	-0.160643	H	0.478907	-0.788309	2.497614
H	0.703694	-0.392274	-1.254386	C	-0.746158	4.028990	-2.454803
C	0.210677	-1.694756	0.287579	H	-2.008930	4.853128	-0.937958
N	-1.012452	-2.172391	-0.032461	H	-2.314056	3.879267	1.269194
N	0.835320	-2.616436	1.002008	H	0.666224	3.000848	-3.750300
N	-0.029355	-3.656623	1.123561	H	-2.556799	3.022652	3.521229
N	-1.138000	-3.406792	0.511645	C	-1.602915	1.253995	4.252681
C	-2.114242	-1.576854	-0.801760	H	-0.465086	-0.543340	4.710224
C	-2.458237	-2.454057	-2.015454	H	-0.945741	4.821123	-3.172133
C	-3.336858	-1.336851	0.099096	H	-2.017130	1.340457	5.254094
H	-1.738558	-0.606572	-1.149644				
C	-3.621762	-1.845352	-2.813320				
H	-2.727410	-3.455198	-1.656292				
H	-1.570572	-2.570680	-2.650182				
C	-4.495686	-0.734421	-0.710466				
H	-3.638452	-2.296927	0.537398				
H	-3.054866	-0.677488	0.928423				
C	-4.850401	-1.605247	-1.923690				
H	-3.876727	-2.506534	-3.650557				
H	-3.301880	-0.891059	-3.258551				
H	-5.369371	-0.609192	-0.059368				
H	-4.217760	0.273902	-1.052207				
H	-5.652248	-1.134779	-2.506438				
H	-5.242335	-2.572631	-1.576511				
H	2.407174	-0.159122	1.098917				
H	6.711544	1.368161	-1.377911				
C	0.009842	0.863575	0.313976				
C	-0.205393	1.915127	-0.615068				

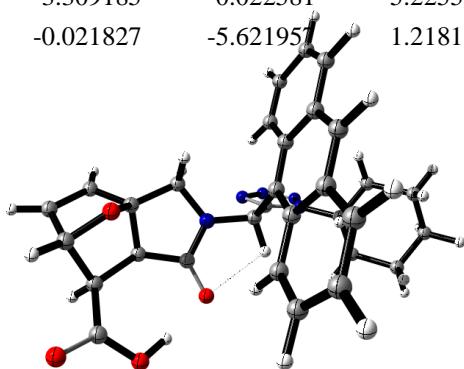


**8j**

E(scf) = -1773.44515245 a.u.

 $\nu_{\min} = 17.0 \text{ cm}^{-1}$ 

C	4.819442	0.527437	0.729955	H	-3.949375	-0.945629	3.205970
C	3.504131	1.328984	0.476299	H	-6.369899	-0.143273	0.357737
C	5.117799	0.052018	-0.745628	H	-5.012217	-1.179828	0.774008
C	5.502372	1.275099	-1.573284	H	-6.389492	-0.770810	2.797374
C	3.303348	1.125094	-1.069860	H	-6.262489	0.971067	2.573743
O	3.788870	-0.213665	-1.210097	H	5.741974	-0.836803	-0.798682
C	1.807372	1.203265	-1.307518	H	3.366232	-0.049168	2.730088
H	1.485748	2.211727	-1.590039	C	-0.682807	-0.612227	-0.587356
N	1.260067	0.847493	0.006686	C	-1.355271	-0.407927	-1.820692
C	4.900349	-0.675544	1.699635	C	-0.488599	-1.929297	-0.085568
C	2.159211	0.880629	1.020950	C	-1.936109	-1.546848	-2.504785
O	4.115311	-0.689520	2.777434	C	-1.491517	0.867378	-2.466632
H	5.602090	1.209095	1.085258	C	-1.064357	-3.052375	-0.793200
H	3.614113	2.383292	0.757036	C	0.270788	-2.226800	1.095274
O	5.735795	-1.525663	1.524873	C	-2.646938	-1.353687	-3.730884
O	1.894097	0.633844	2.200458	C	-1.787986	-2.826411	-1.966271
C	4.362451	1.939175	-1.795398	C	-2.170134	1.007141	-3.650718
H	4.213538	2.906188	-2.262681	H	-1.036276	1.749733	-2.033806
H	6.514606	1.569814	-1.826663	C	-0.887061	-4.378213	-0.288582
H	1.489329	0.484674	-2.068125	C	0.430084	-3.516015	1.537750
C	-0.142786	0.542051	0.268959	H	0.772082	-1.438709	1.648038
H	-0.138982	0.197968	1.309366	C	-2.770271	-0.111814	-4.291199
C	-0.960769	1.812049	0.301335	H	-3.080637	-2.226090	-4.215705
N	-2.237418	1.911053	0.724571	H	-2.233169	-3.673837	-2.485871
N	-0.526201	3.020945	-0.007994	H	-2.243235	1.990613	-4.108448
N	-1.566152	3.863550	0.226217	H	-1.336381	-5.202815	-0.838392
N	-2.593229	3.216750	0.665854	C	-0.160334	-4.609661	0.847392
C	-3.171836	0.892376	1.227381	H	1.032114	-3.701920	2.423540
C	-3.448442	1.106799	2.724550	H	-3.309185	0.022581	-5.225509
C	-4.465417	0.882897	0.398207	H	-0.021827	-5.621951	1.218115
H	-2.658451	-0.067491	1.088441				
C	-4.426586	0.044852	3.249086				
H	-3.868614	2.111632	2.860950				
H	-2.504594	1.075658	3.283346				
C	-5.438071	-0.178047	0.935066				
H	-4.922102	1.879111	0.451741				
H	-4.223444	0.694415	-0.654472				
C	-5.725585	0.021772	2.430409				
H	-4.642336	0.237338	4.306920				

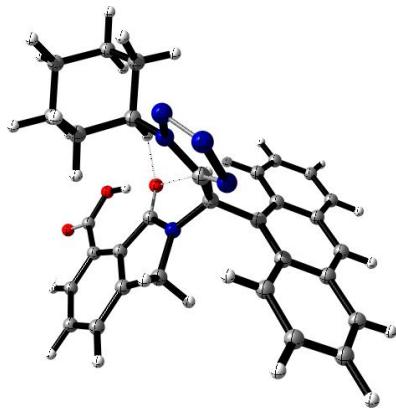


**1j**

E(scf) = -1697.06261954 a.u.

ν<sub>min</sub> = 11.28 cm<sup>-1</sup>

C	2.970485	-2.821679	0.232751	C	3.870582	-2.564497	1.438196
C	1.842079	-2.088950	-0.192087	O	4.818147	-3.283339	1.643806
C	3.337950	-3.918189	-0.558336	O	3.599351	-1.536774	2.236411
C	2.632352	-4.271779	-1.710943	H	2.779191	-1.035126	1.994238
C	1.144086	-2.441868	-1.353456	C	-2.191325	0.158905	0.260692
C	0.002232	-1.488327	-1.573798	C	-3.161640	-0.289901	-0.677116
H	0.091901	-0.951497	-2.527440	C	-2.513516	0.209338	1.650593
N	0.127352	-0.570233	-0.446349	C	-4.475242	-0.683751	-0.209269
C	1.163592	-0.897854	0.380350	C	-2.938250	-0.395116	-2.089885
O	1.460623	-0.272673	1.407123	C	-3.853618	-0.134762	2.082245
C	1.523654	-3.532182	-2.126879	C	-1.593235	0.576285	2.692535
H	0.976859	-3.803373	-3.026830	C	-5.451975	-1.171549	-1.133669
H	2.956512	-5.132057	-2.290763	C	-4.788007	-0.574678	1.145164
H	-0.970594	-1.992826	-1.559158	C	-3.897874	-0.870879	-2.945780
C	-0.762214	0.566677	-0.133302	H	-2.010967	-0.038173	-2.512961
H	-0.306316	0.957596	0.775405	C	-4.214098	-0.039875	3.462880
C	-0.599893	1.702398	-1.126347	C	-1.974788	0.644542	4.008448
N	0.500416	2.500967	-1.167810	H	-0.547214	0.763085	2.476112
N	-1.450491	2.140007	-2.037183	C	-5.174249	-1.275366	-2.468046
N	-0.858798	3.197481	-2.641376	H	-6.426687	-1.459116	-0.744722
N	0.309378	3.421323	-2.133448	H	-5.787271	-0.847355	1.481687
C	1.754607	2.488722	-0.396531	H	-3.684555	-0.917782	-4.011034
C	2.920414	1.979936	-1.260755	H	-5.234378	-0.293069	3.743924
C	2.050023	3.875937	0.194546	C	-3.306044	0.349383	4.407691
H	1.596339	1.784761	0.427106	H	-1.237885	0.918030	4.759698
C	4.218962	1.945410	-0.439743	H	-5.922735	-1.647036	-3.163181
H	3.031114	2.646730	-2.125994	H	-3.588390	0.417711	5.455015
H	2.684330	0.981746	-1.652494				
C	3.350761	3.834685	1.012567				
H	2.135526	4.601622	-0.623017				
H	1.207527	4.196290	0.820153				
C	4.530208	3.317524	0.175678				
H	5.047550	1.614560	-1.077399				
H	4.125339	1.196675	0.360178				
H	3.568145	4.836540	1.402101				
H	3.212549	3.183767	1.888325				
H	5.433355	3.255264	0.794823				
H	4.749348	4.036490	-0.627595				
H	4.205310	-4.489199	-0.242113				



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